The identity of the Hubbard Model upon cooling – Cluster dynamical mean-field and quantum Monte Carlo perspective

Thomas A. Maier

Oak Ridge National Laboratory

2020 Aspen Winter Conference on Computation Meets Experiment – March 9, 2020

ORNL is managed by UT-Battelle, LLC for the US Department of Energy

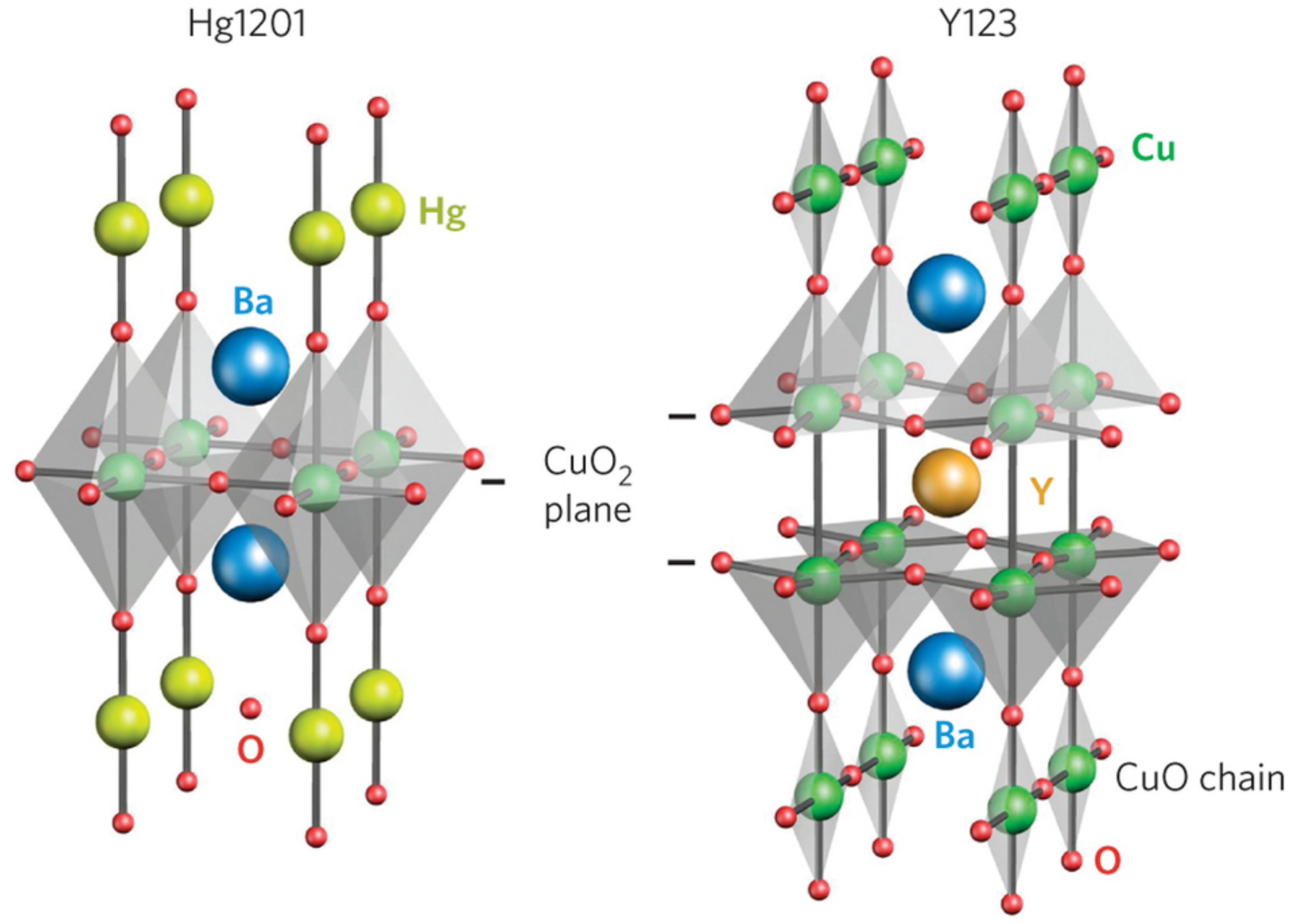
This work was supported by the Scientific Discovery through Advanced Computing (SciDAC) program funded by U.S. Department of Energy, Office of Science, Advanced Scientific Computing Research and Basic Energy Sciences, Division of Materials Sciences and Engineering.

Outline

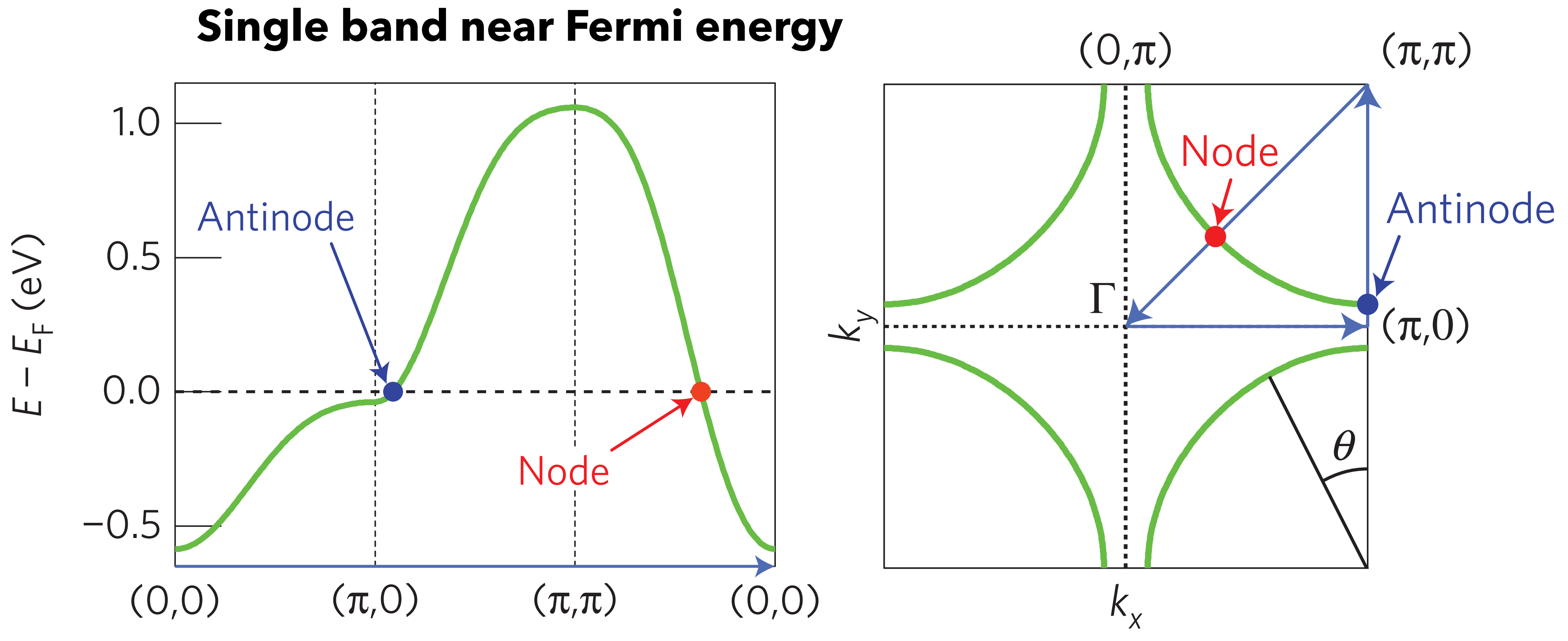
Is the Hubbard model superconducting?

How does superconductivity arise in the presence of a pseudogap?

Cuprates and the Hubbard Model



from Barišić et al., Nat. Phys. 2013



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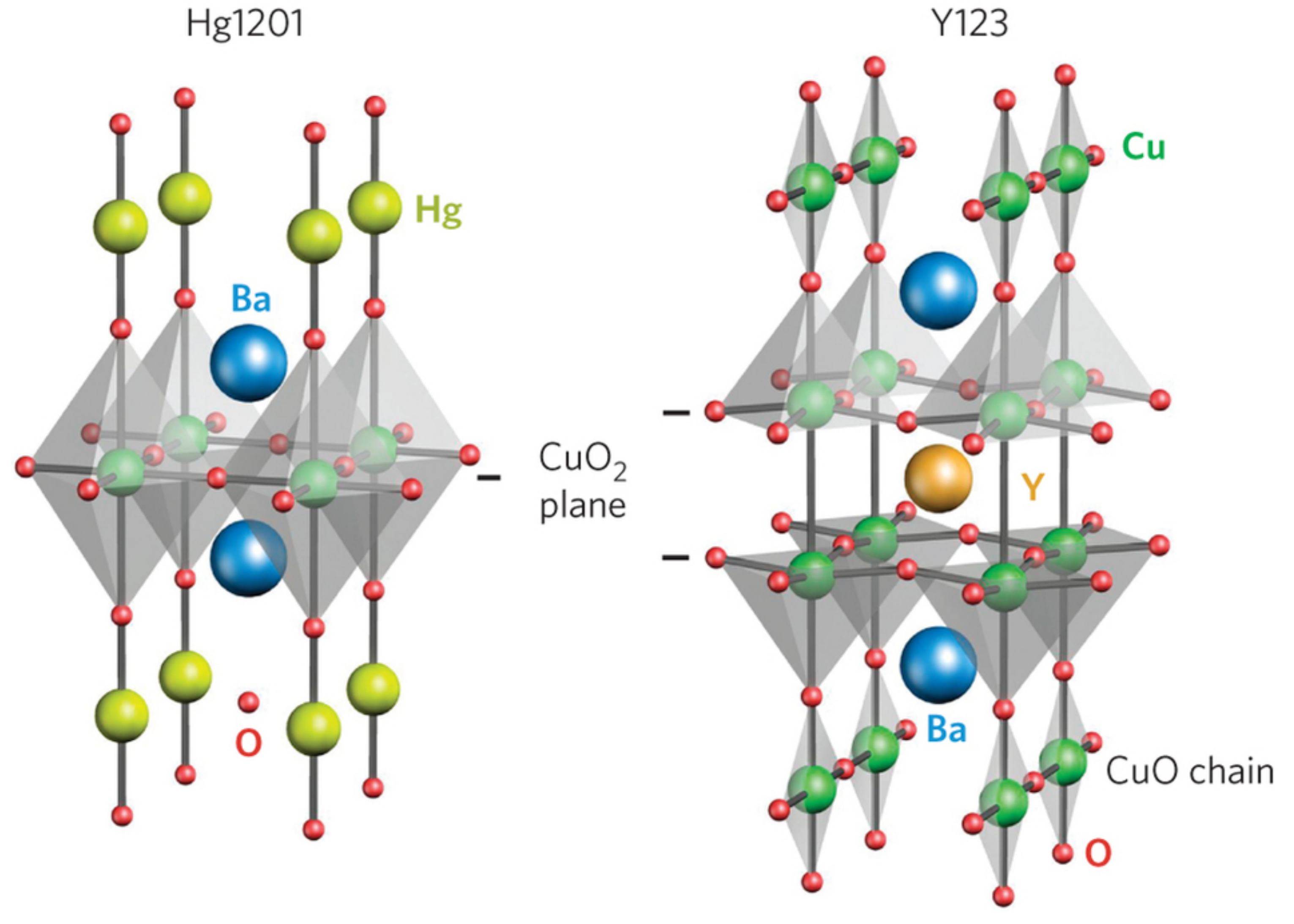

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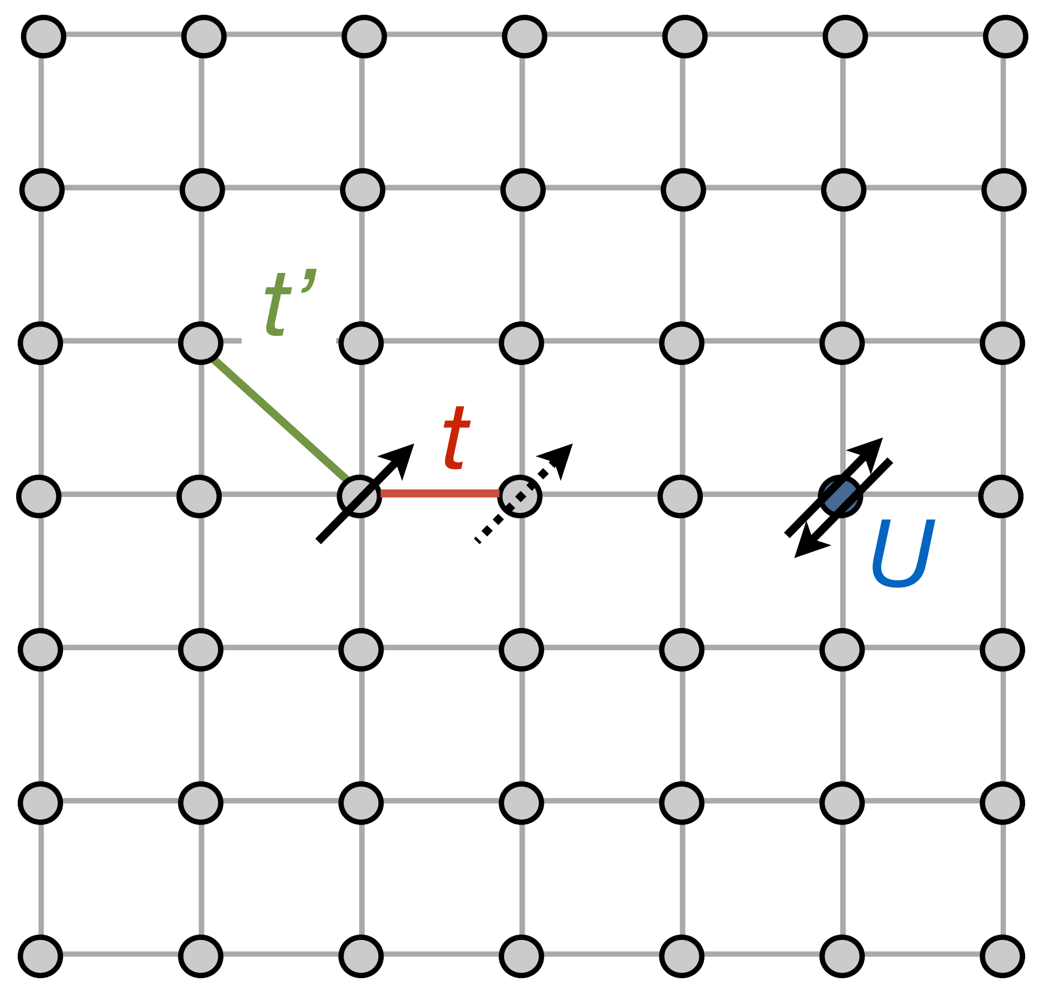
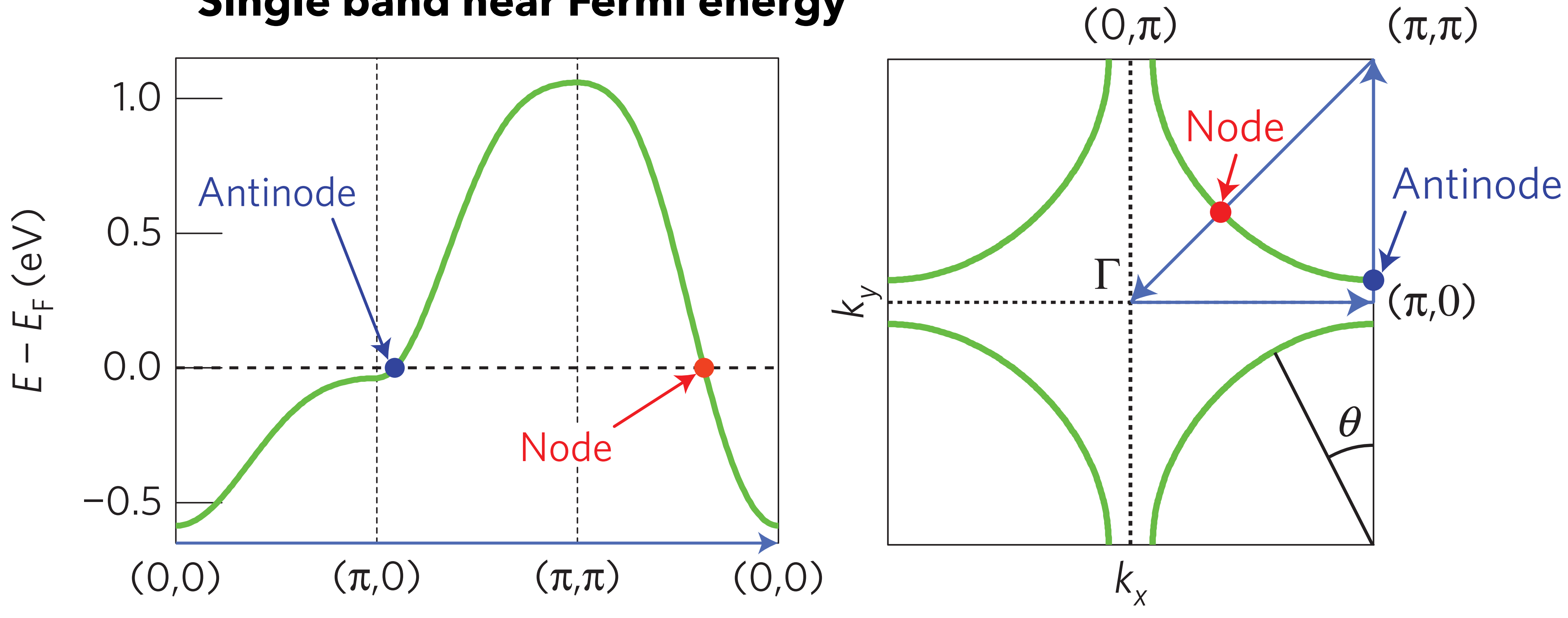


$$\mathcal{H} = \sum_{ij,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Parameters:

- ***t*** : nearest neighbor hopping
- ***t'*** : next-nearest neighbor hopping
- ***U*** : On-site Coulomb repulsion

Single band near Fermi energy



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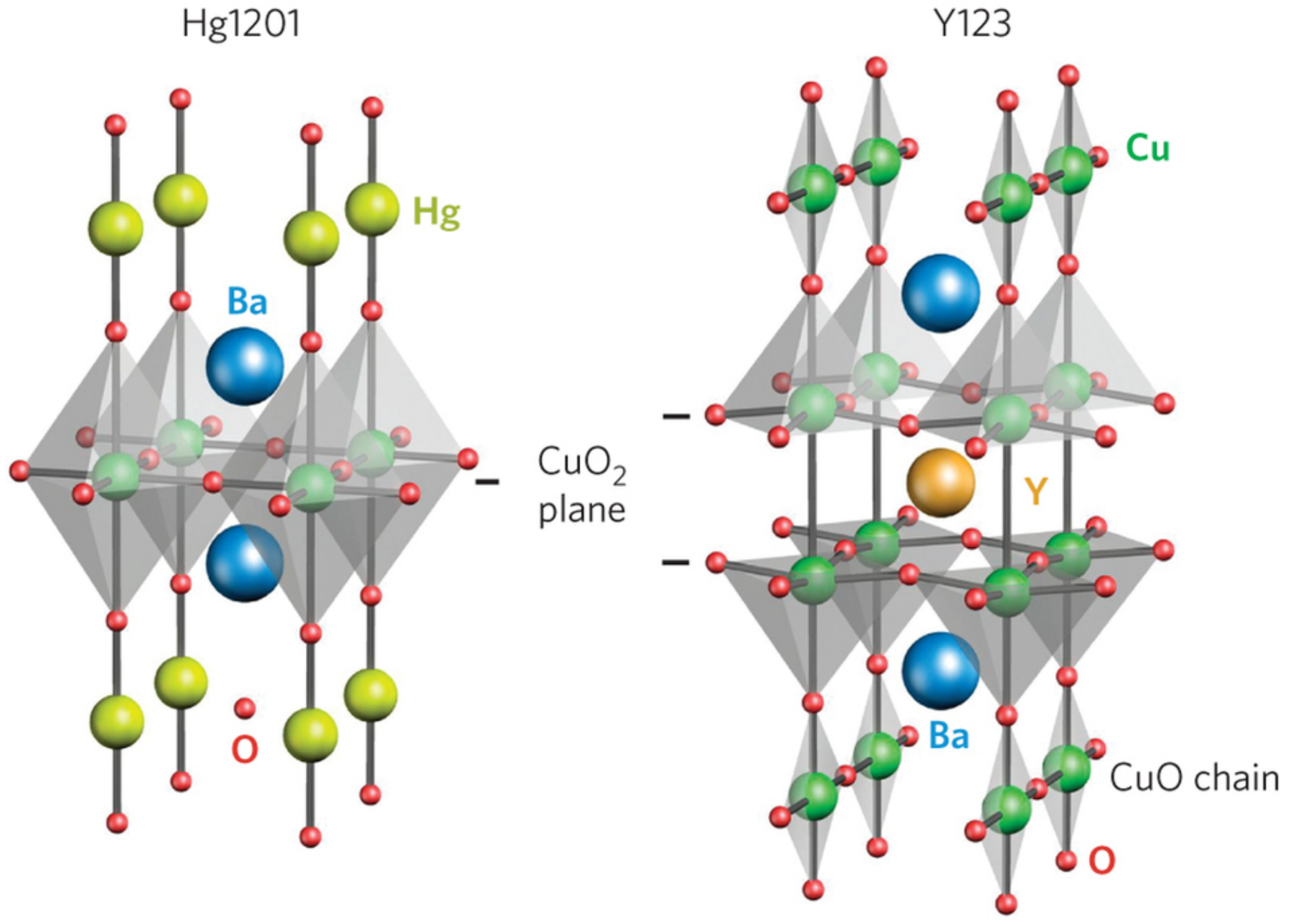

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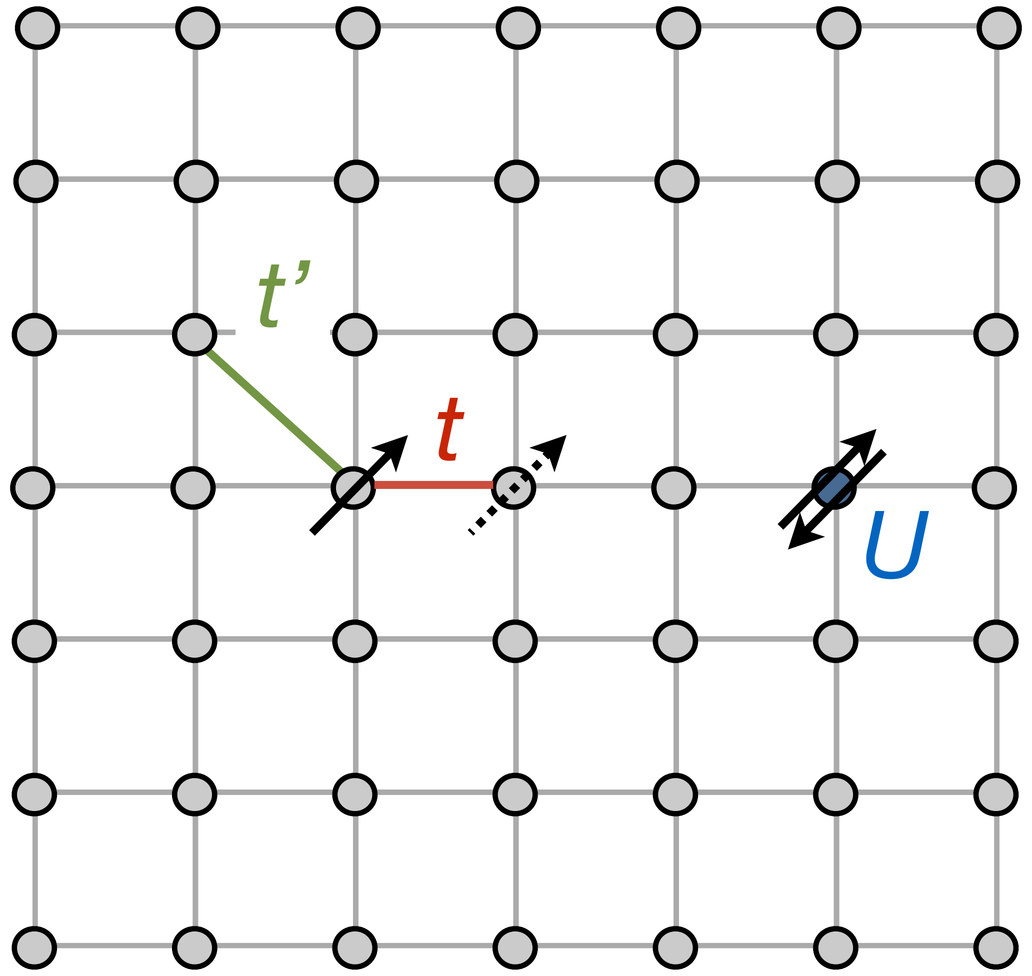

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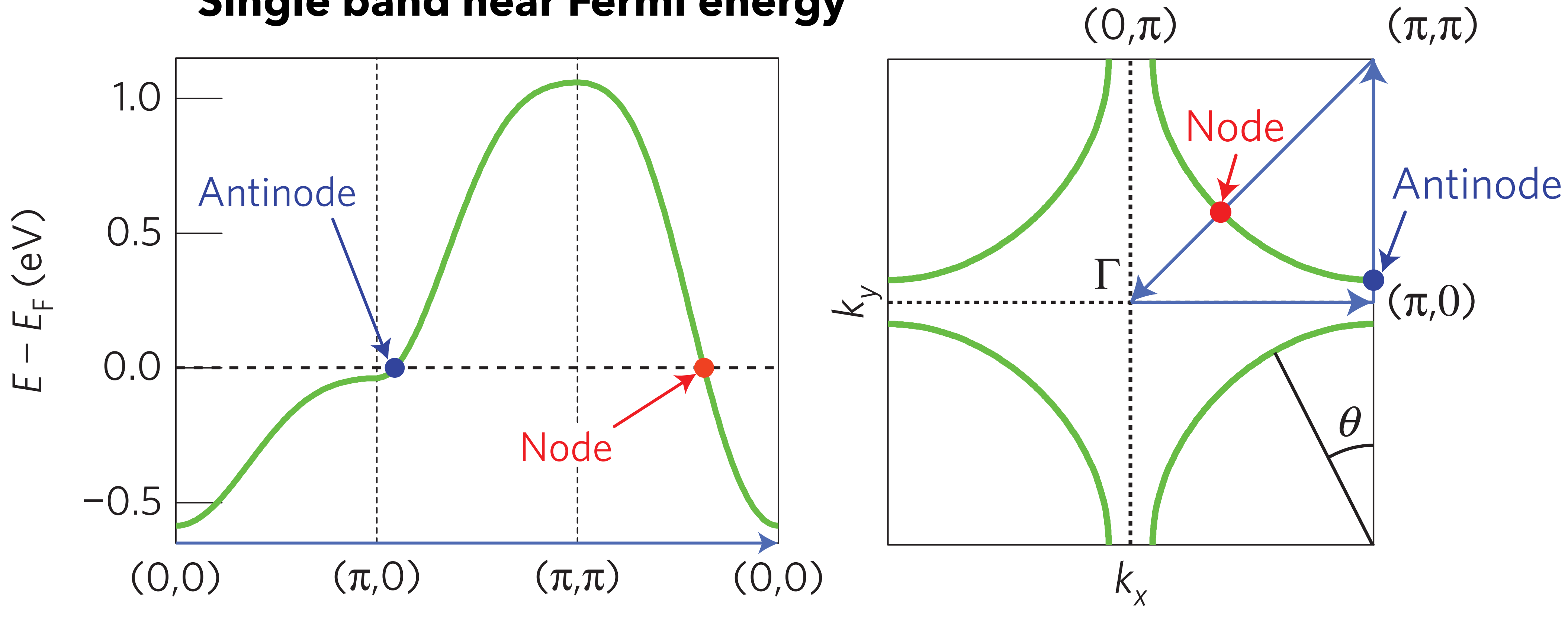

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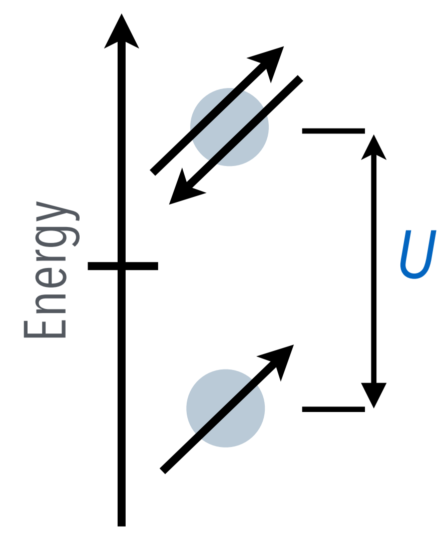
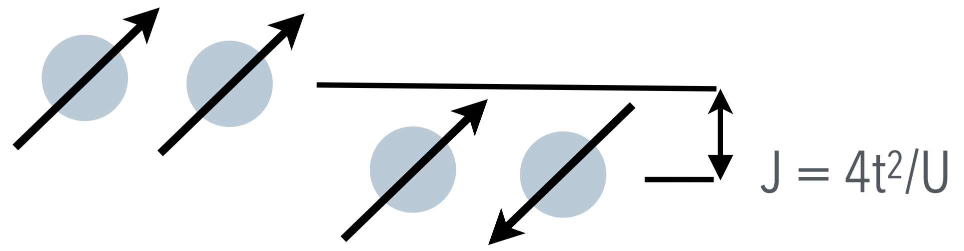
Moment formation



Antiferromagnetic exchange



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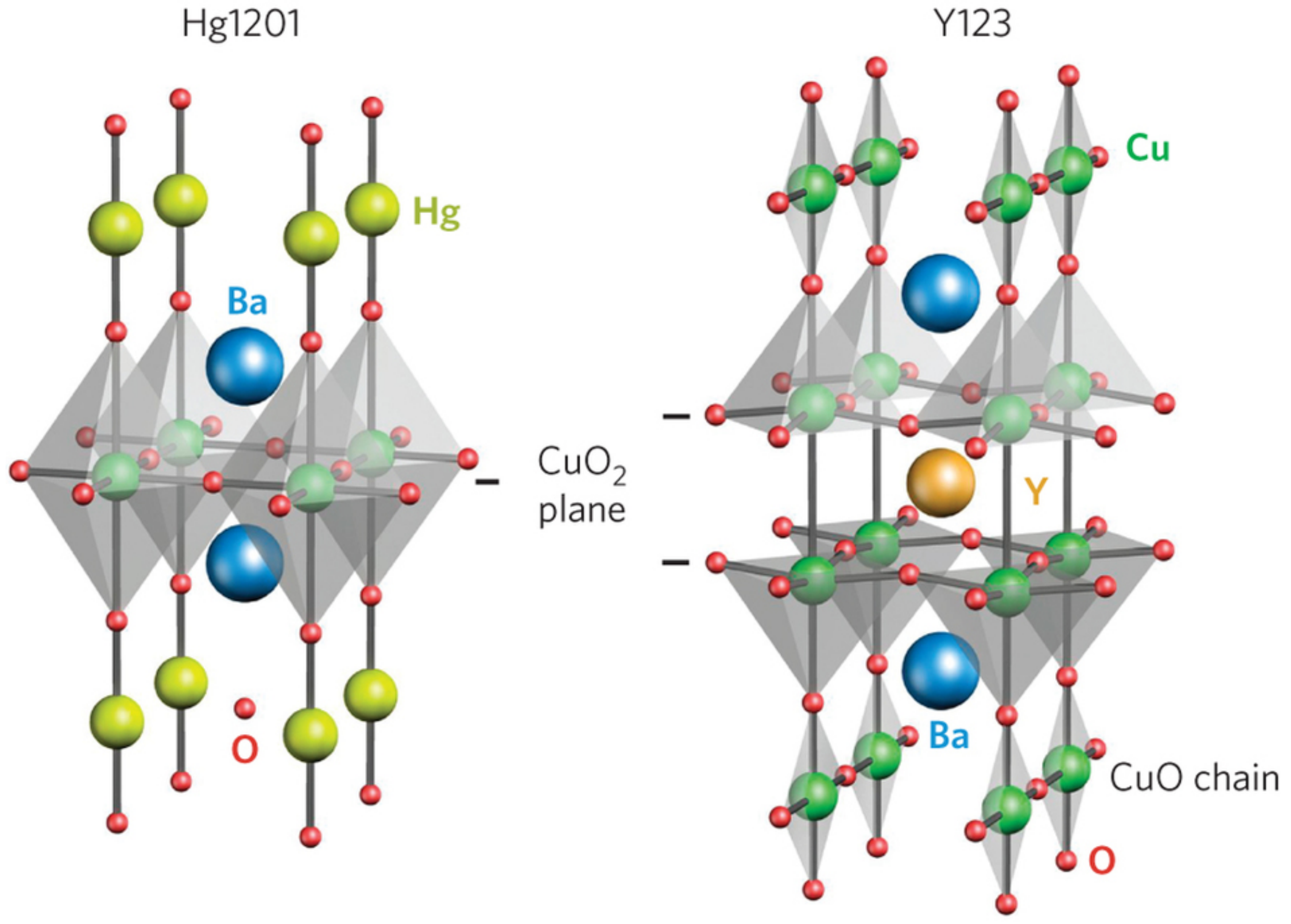

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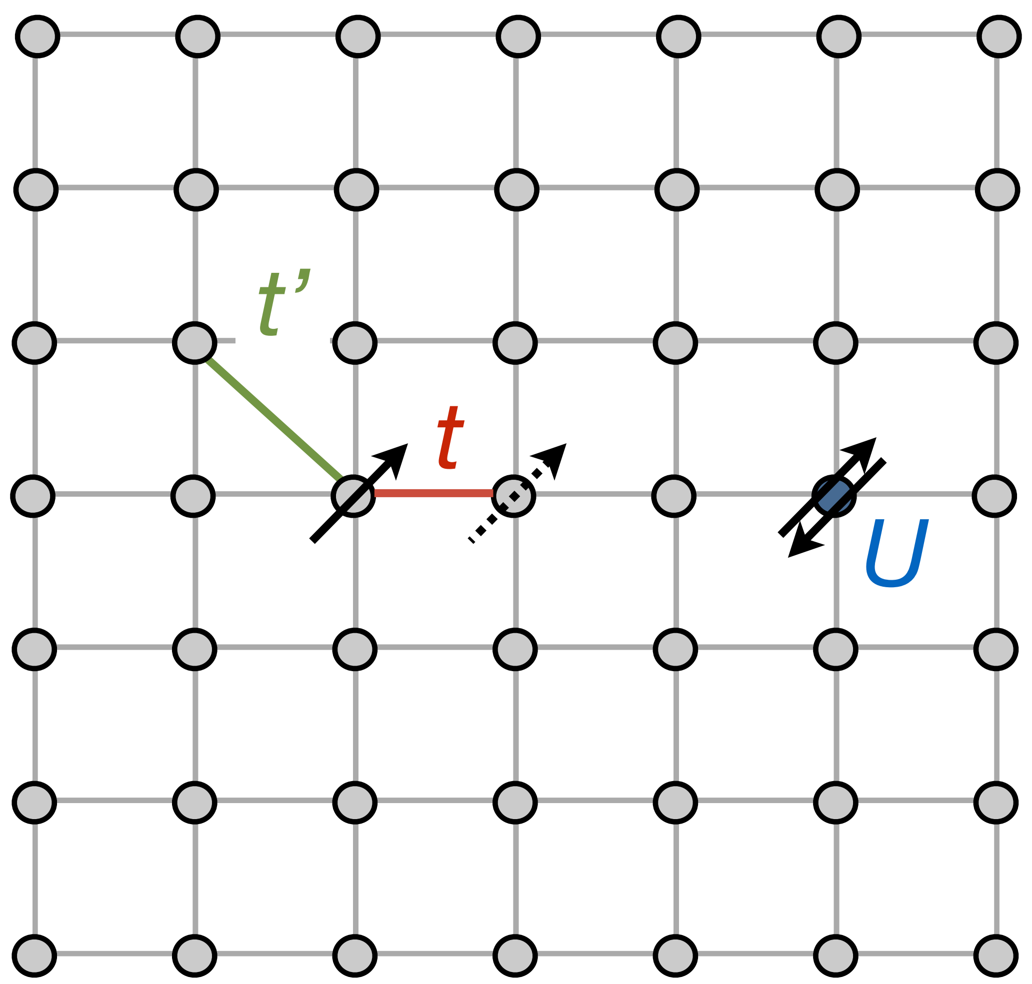

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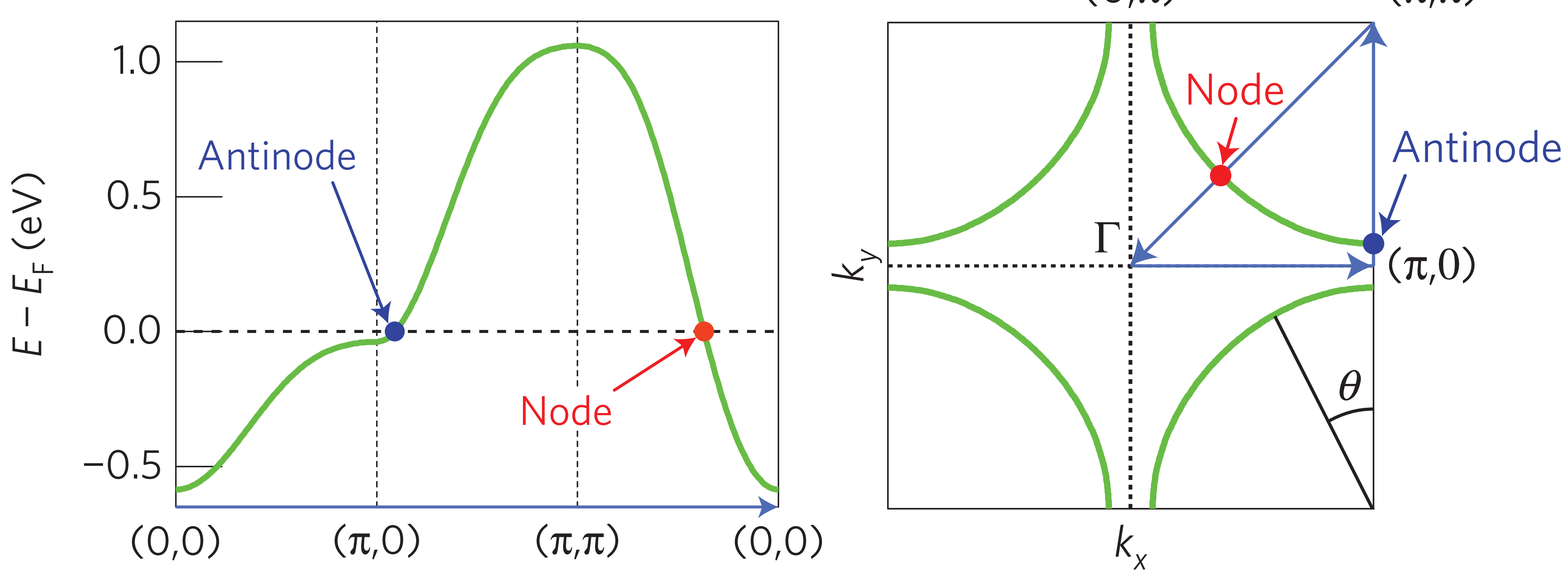

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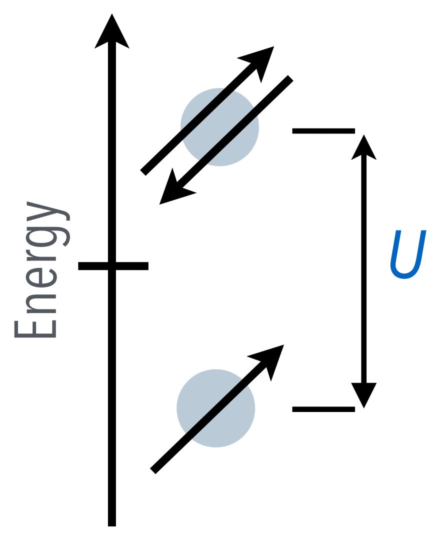
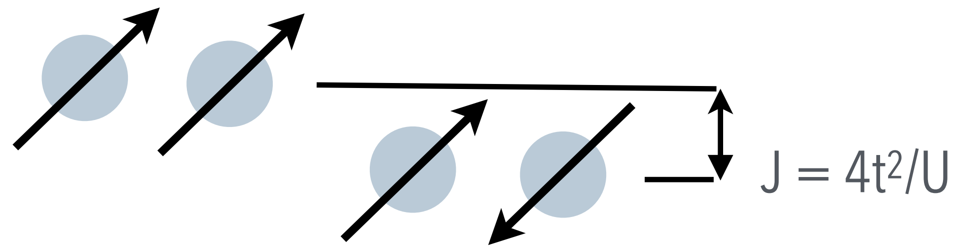
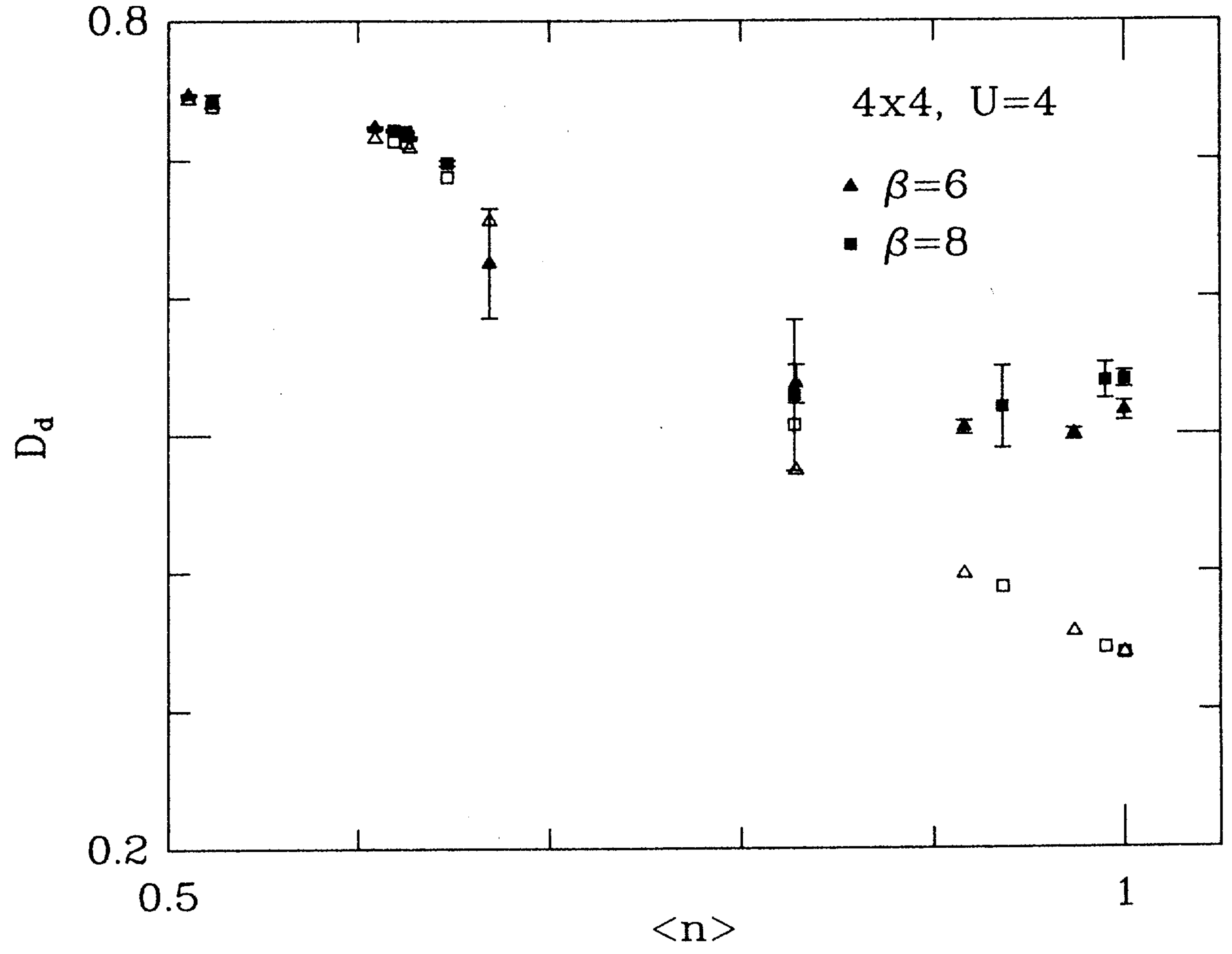




Does the Hubbard model have a superconducting state?

Pairing in the Hubbard model: Pre – Quantum Cluster Period

d-wave pair-field susceptibilty



1989

DQMC on
4 x 4 Hubbard lattice
with *U*=4*t*
White et al., PRB '89

Pair-field susceptibility

$$P_d = \int_0^\infty d\tau \, \langle \mathcal{T}_\tau \Delta_d(\tau) \Delta_d^\dagger(0) \rangle$$

$$\Delta_d^\dagger = \sum_k (\cos k_x - \cos k_y) \, c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger$$

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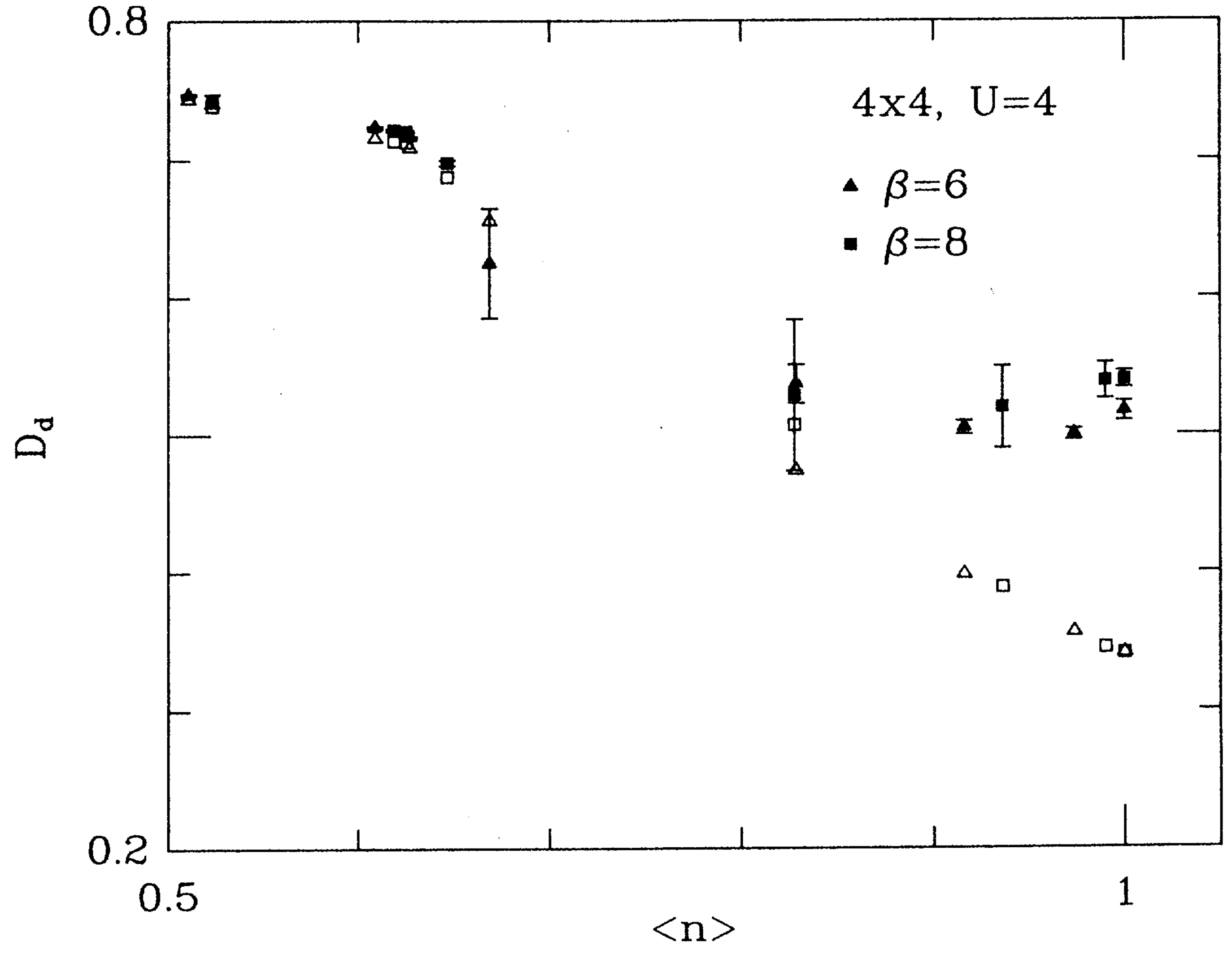

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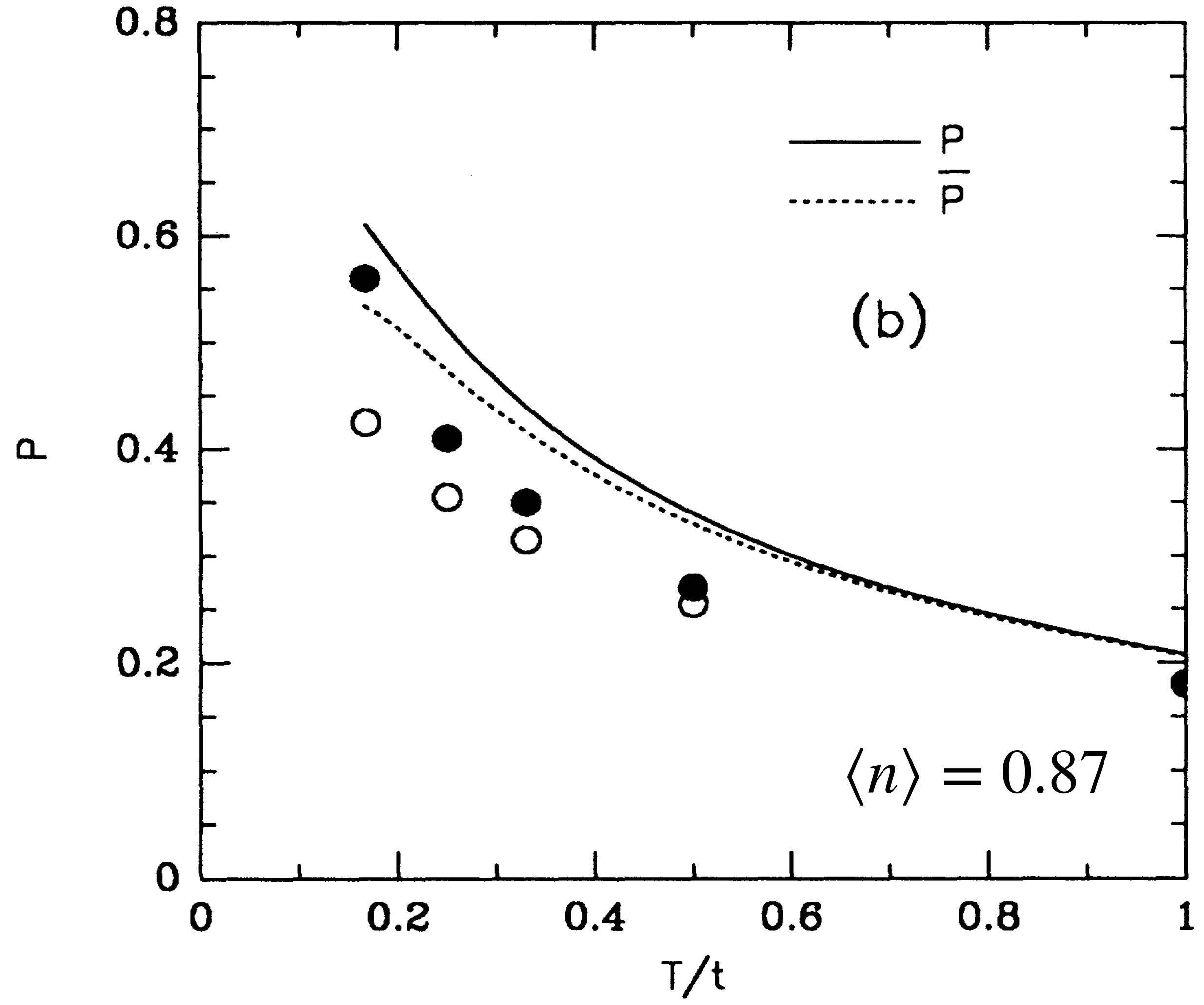

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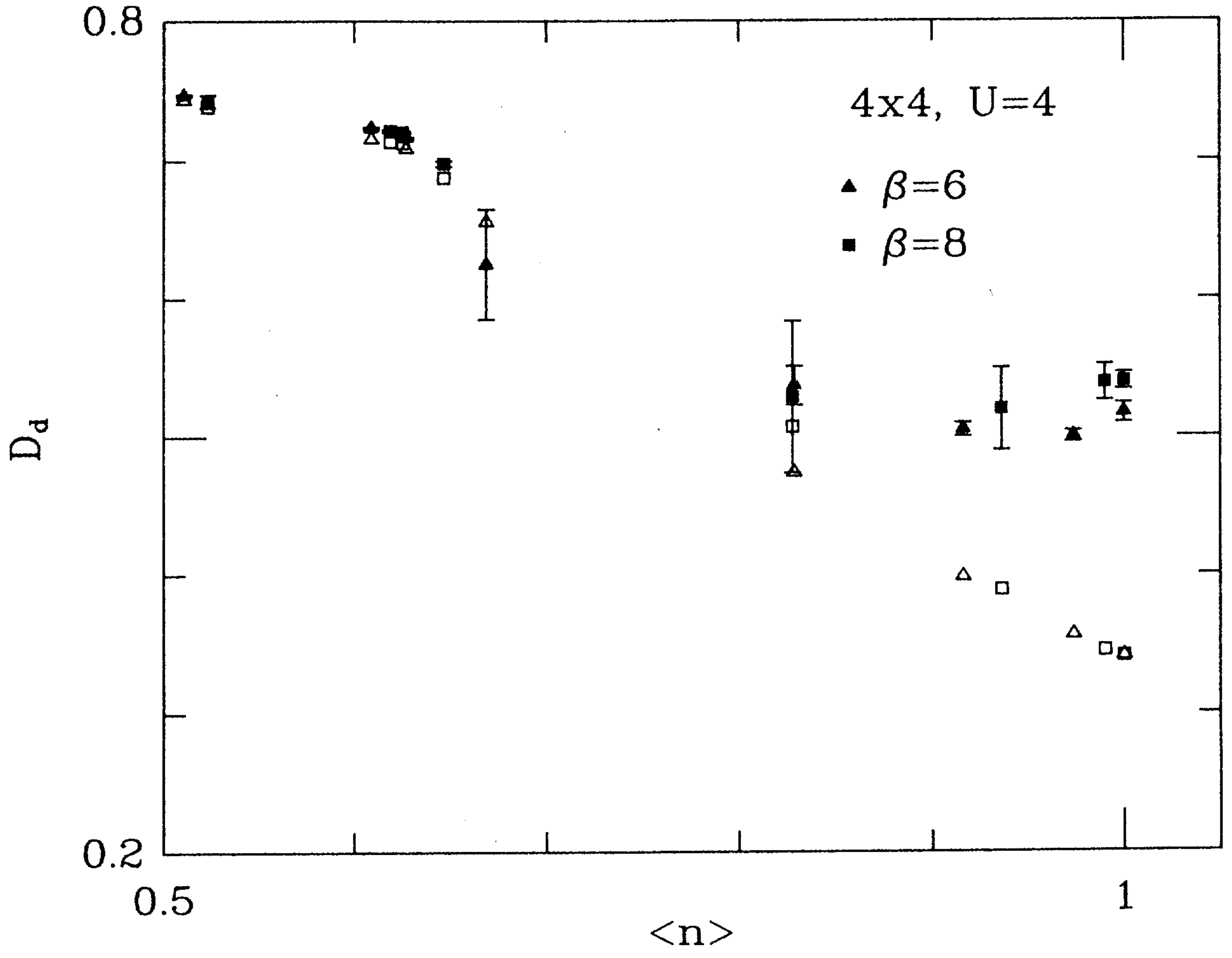

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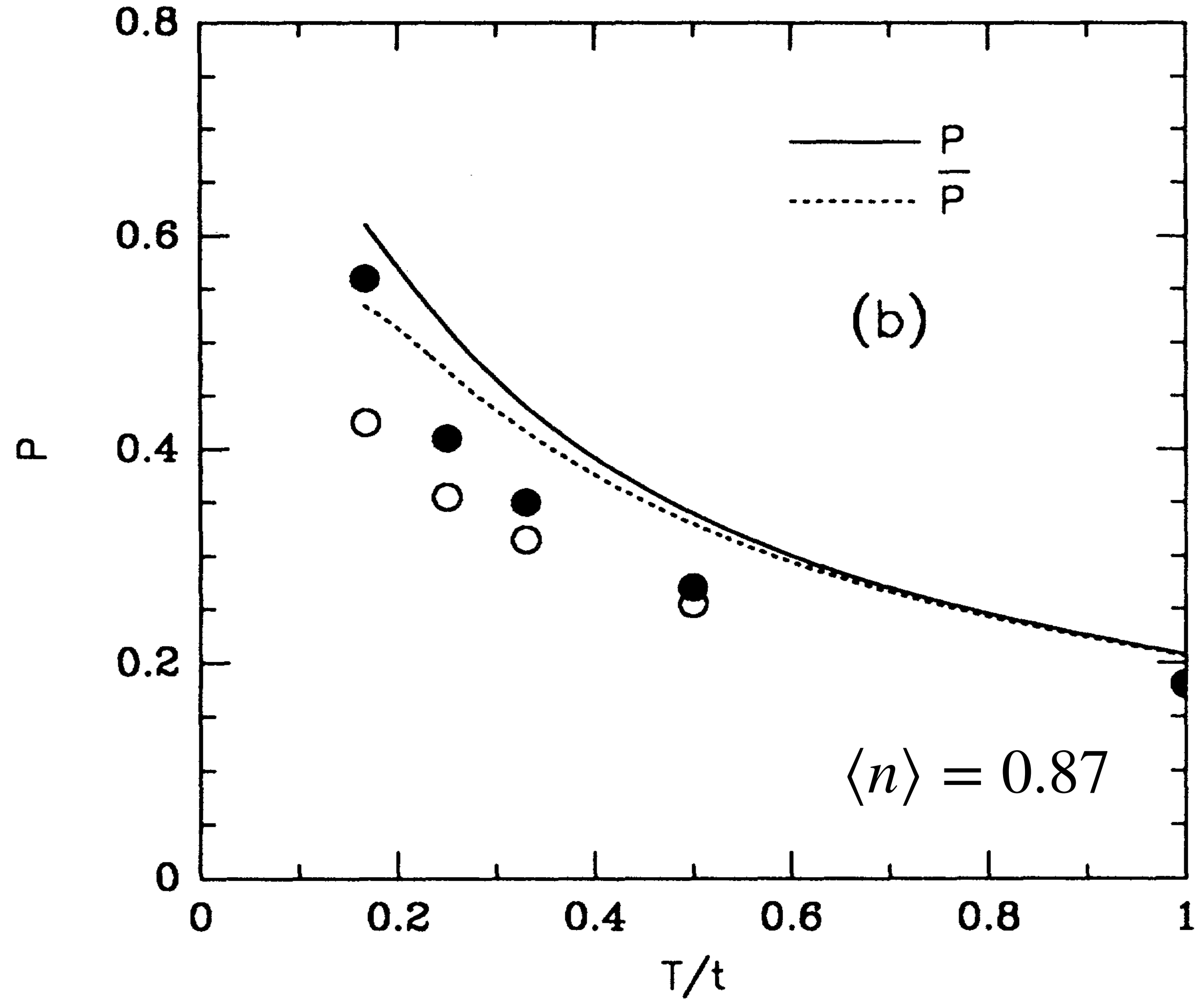

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QMC sign problem prevents calculations at sufficiently low temperatures

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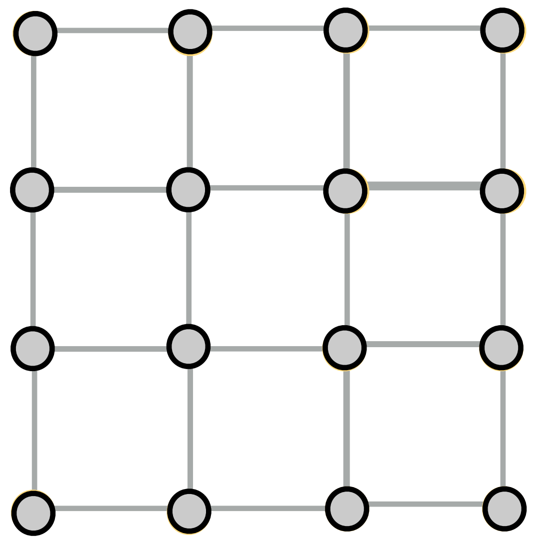
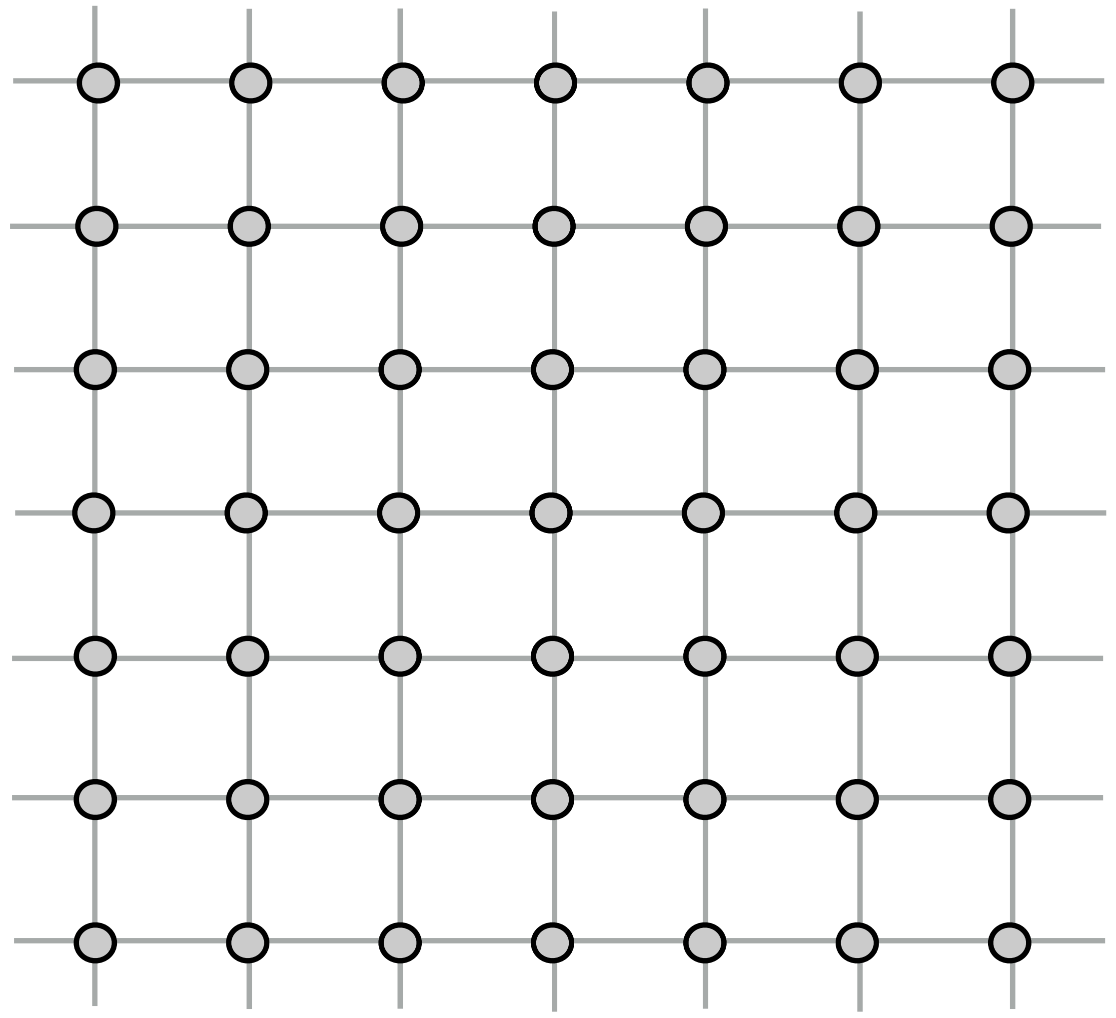
Quantum Cluster Theories

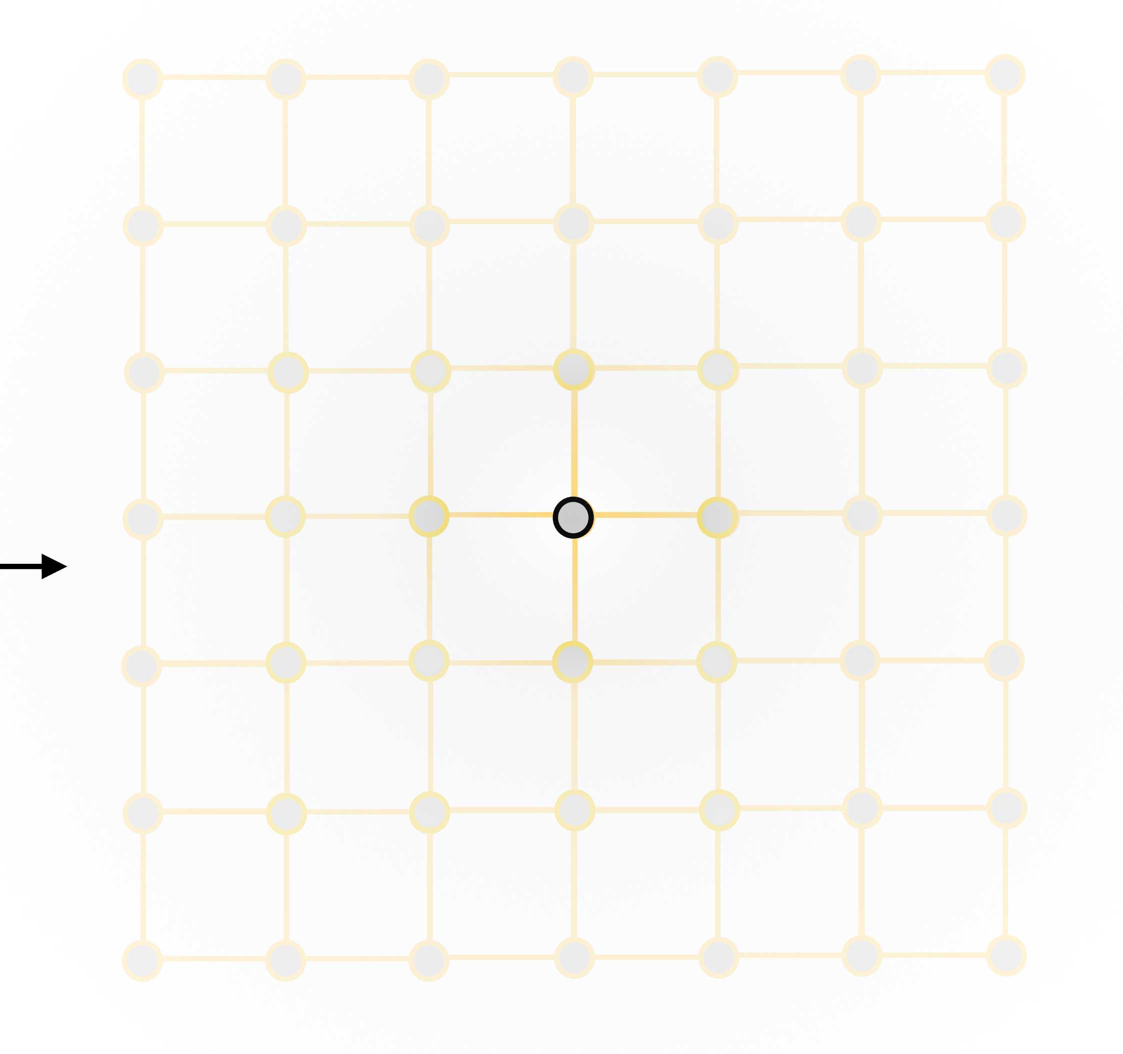
Finite size approximations
(ED, DMRG, **DQMC**, …)





Dynamical mean field theory

Metzner & Vollhardt, PRL ’89
Müller-Hartmann, Z. Phys. B ’89
Georges et al., RMP ’96



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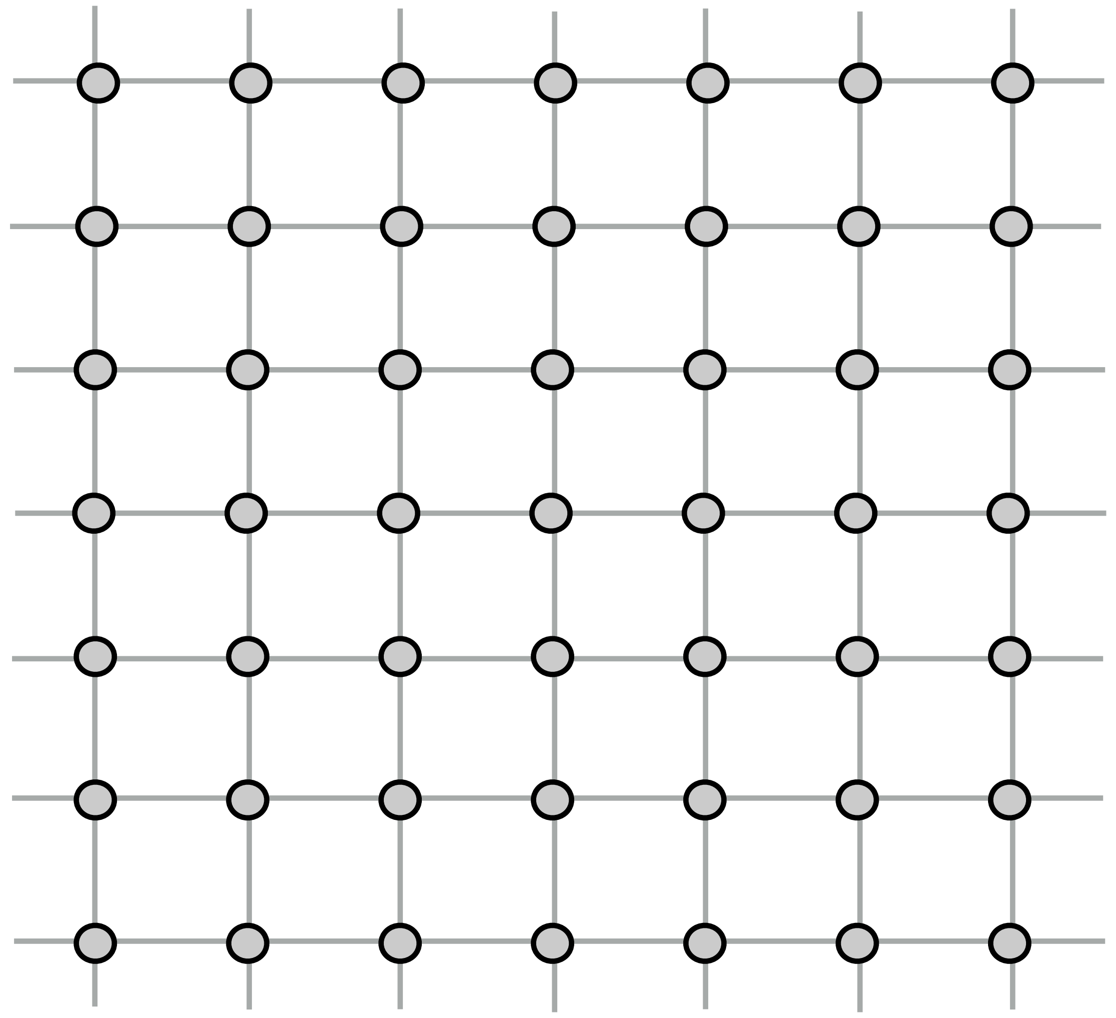

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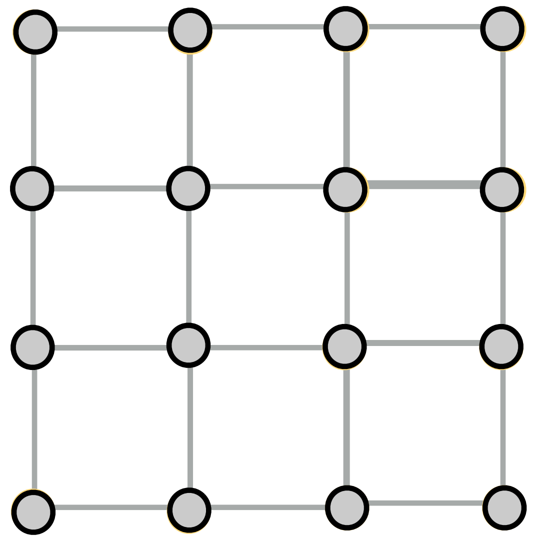
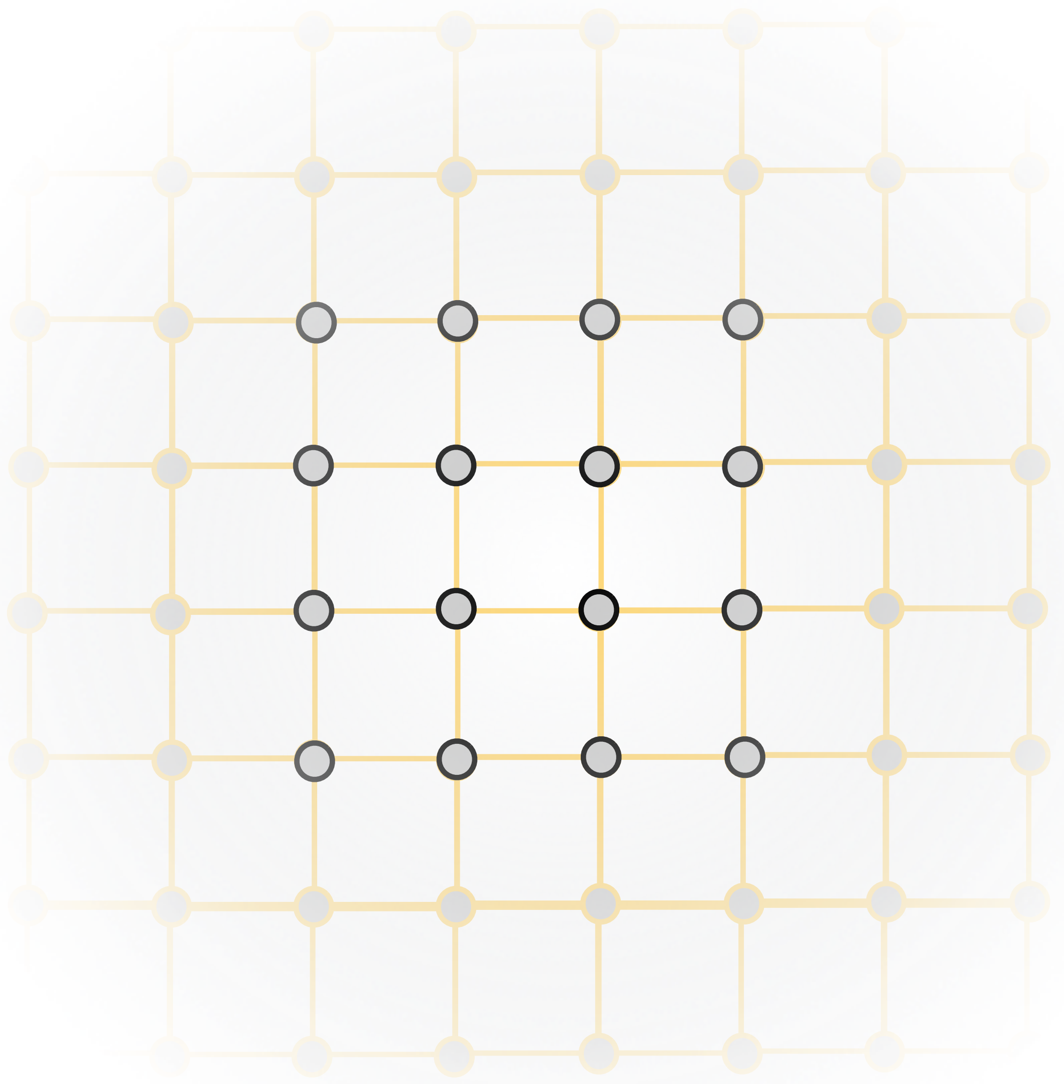


Quantum cluster theories

(**DCA**, CDMFT, CPT, VCA, …)



Hettler et al., PRB ’98
Liechtenstein & Katsnelson, PRB ’00
Kotliar et al., PRL ’01
TAM, Hettler, Pruschke & Jarrell, RMP ’05

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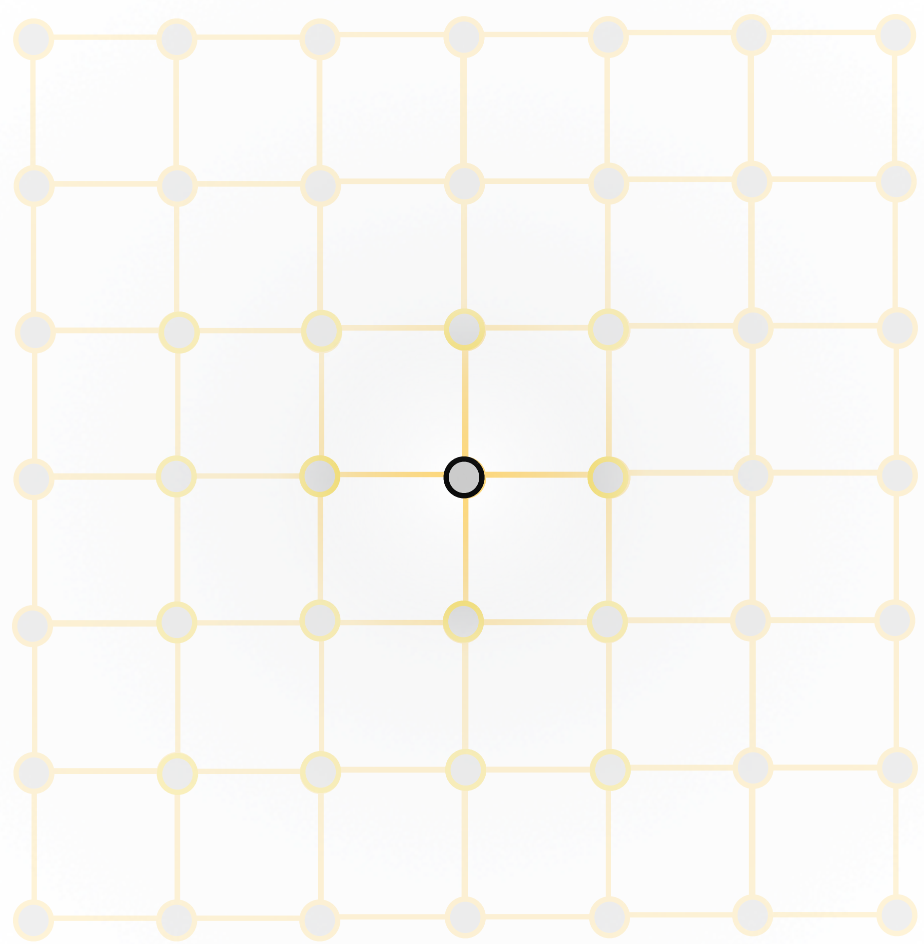
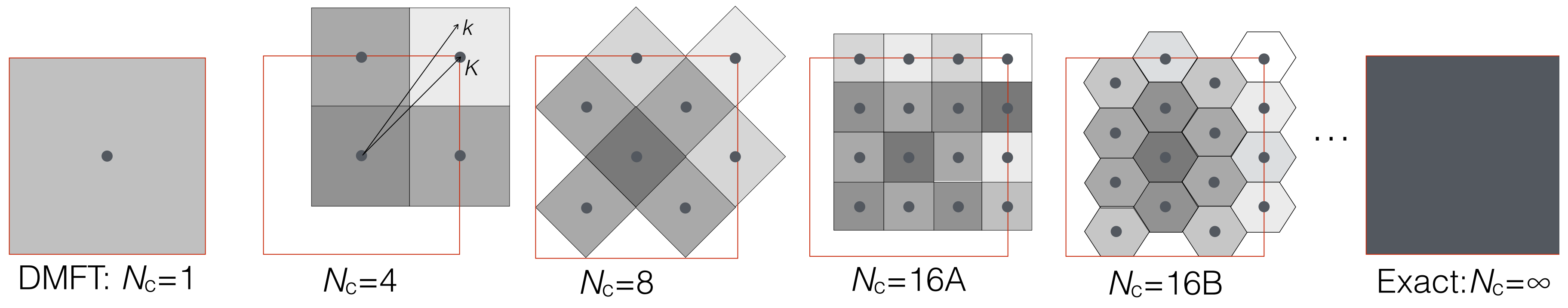
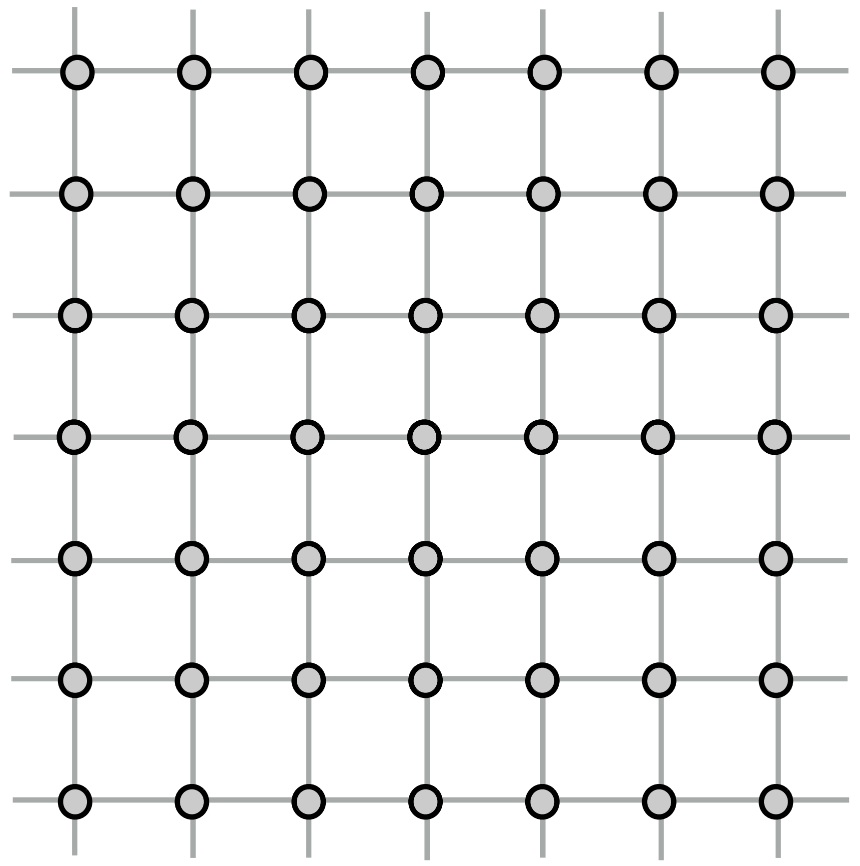


Dynamical Cluster Approximation

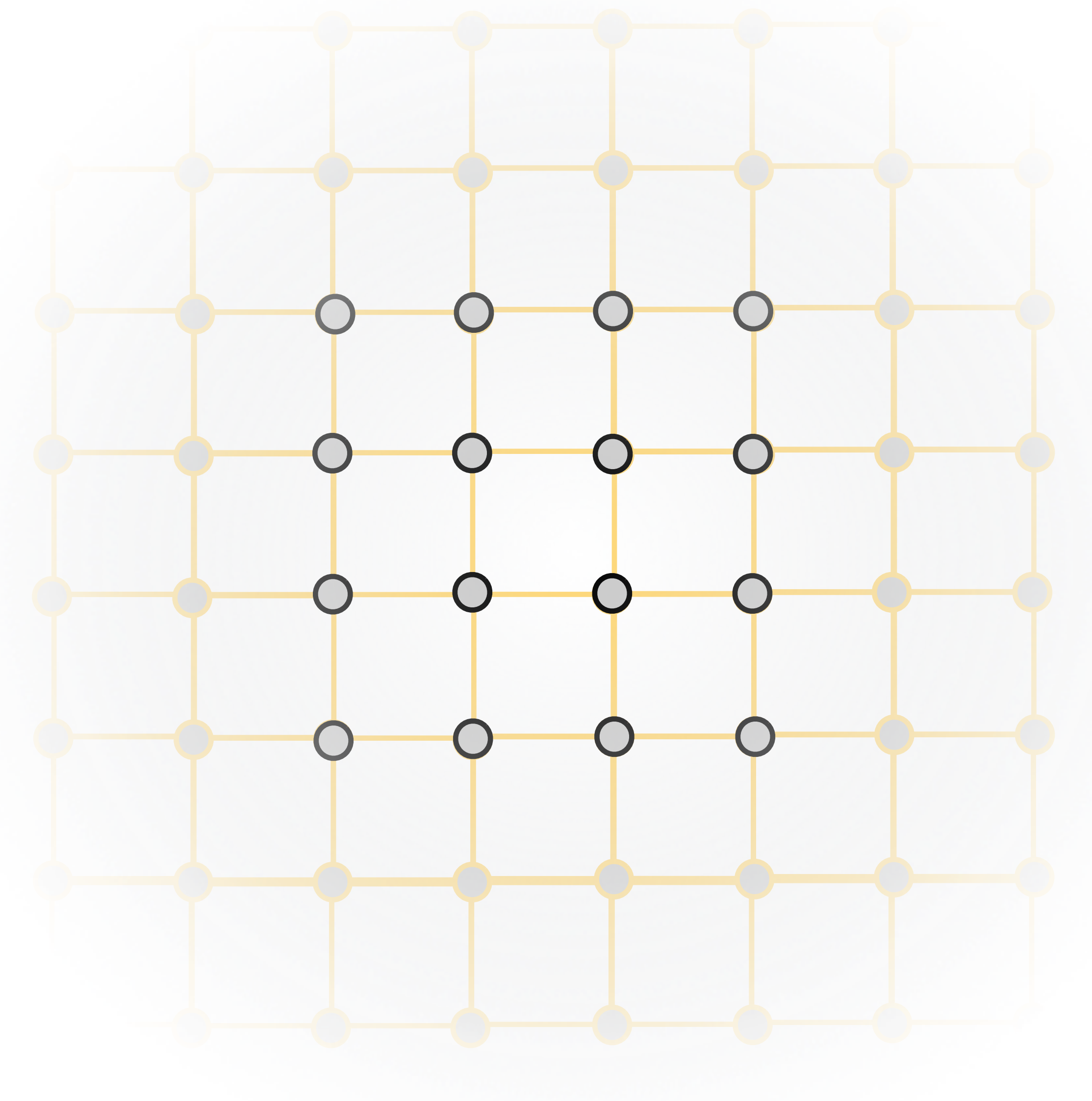


Infinite size lattice



DCA self-consistently maps infinite size lattice to **effective cluster embedded in dynamic mean-field** that describes the remaining lattice degrees of freedom

Cluster embedded in mean-field



(1) Coarse-graining

$$\bar{G}(\mathbf{K}, i\omega_n) = \frac{N_c}{N}\sum_{\mathbf{k}\in\mathscr{P}_\mathbf{K}} G(\mathbf{k}, i\omega_n) = \frac{N_c}{N}\sum_{\mathbf{k}\in\mathscr{P}_\mathbf{K}} \frac{1}{i\omega_n - \varepsilon_\mathbf{k} + \mu - \Sigma_c(\mathbf{K}, i\omega_n)}$$

(2) Cluster exclusion

$$\mathscr{G}_0(\mathbf{K}, i\omega_n) = \left[\bar{G}^{-1}(\mathbf{K}, i\omega_n) + \Sigma_c(\mathbf{K}, i\omega_n)\right]^{-1}$$

$\mathscr{G}_0(\mathbf{K}, i\omega_n)$, U

(3) Quantum Monte Carlo cluster solver

$$S[\phi^*, \phi] = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_{ij,\sigma} \phi^*_{i\sigma}(\tau)\mathscr{G}_{0,ij,\sigma}(\tau-\tau')\phi_{j\sigma}(\tau) + \int_0^\beta d\tau \sum_i U\phi^*_{i\uparrow}(\tau)\phi_{i\uparrow}\phi^*_{i\downarrow}(\tau)\phi_{i\downarrow}(\tau)$$

$$G_{c,ij,\sigma}(\tau-\tau') = \frac{1}{Z}\int \mathscr{D}[\phi^*\phi]\phi_{i\sigma}(\tau)\phi^*_{j\sigma}(\tau')e^{-S[\phi^*,\phi]}; \quad Z = \int \mathscr{D}[\phi^*\phi]e^{-S[\phi^*,\phi]}$$

$G_c(\mathbf{K}, i\omega_n)$

(4) New self-energy

$$\Sigma_c(\mathbf{K}, i\omega_n) = \mathscr{G}_0^{-1}(\mathbf{K}, i\omega_n) - G_c^{-1}(\mathbf{K}, i\omega_n)$$

Numerically exact solution of effective cluster problem with ***quantum Monte Carlo***

Hettler, Tahvildar-Zadeh, Jarrell, Pruschke, Krishnamurthy, PRB '98

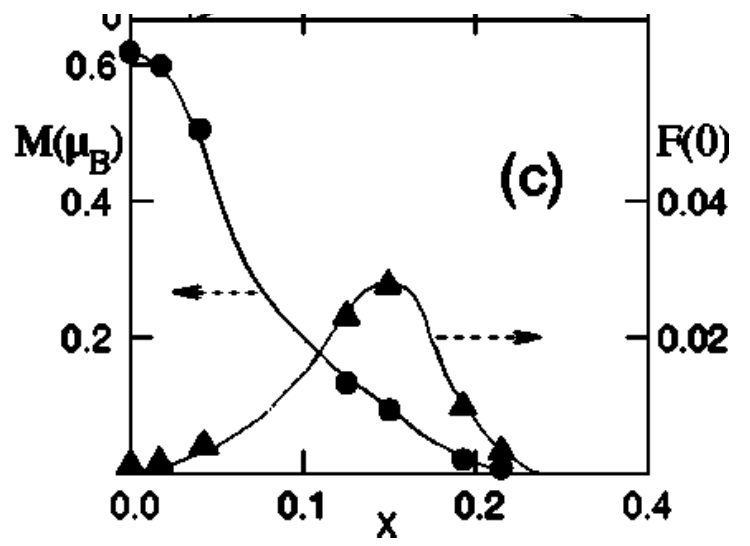
Maier, Jarrell, Pruschke, Hettler, RMP '05

Quantum cluster theory of superconductivity in the Hubbard model

PHYSICAL REVIEW B VOLUME 62, NUMBER 14 1 OCTOBER 2000-II

Antiferromagnetism and *d*-wave superconductivity in cuprates: A cluster dynamical mean-field theory

A. I. Lichtenstein[1] and M. I. Katsnelson[2]



2000

First quantum cluster 2x2 calculations

VOLUME 85, NUMBER 7 PHYSICAL REVIEW LETTERS 14 AUGUST 2000

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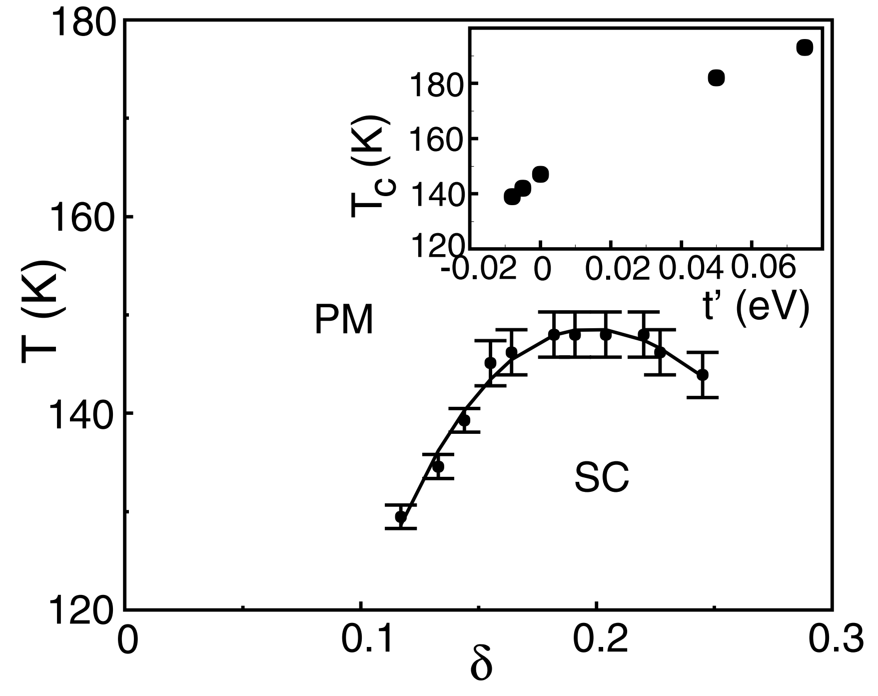

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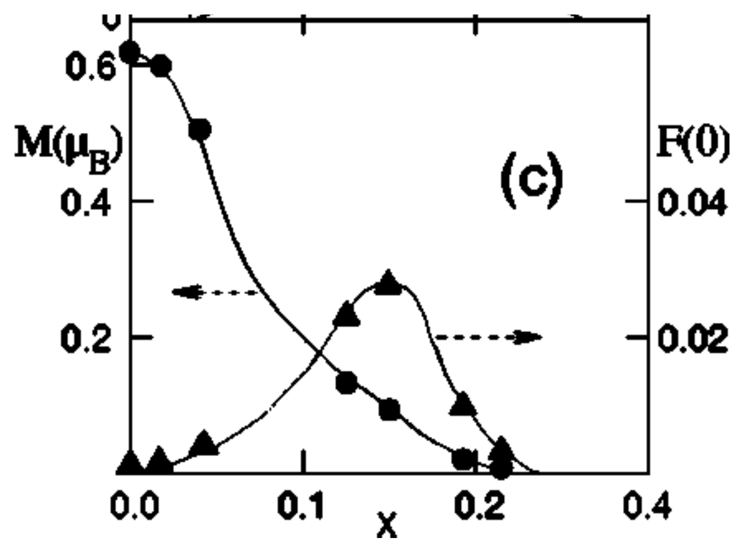

EUROPHYSICS LETTERS 15 November 2001
Europhys. Lett., **56** (4), pp. 563–569 (2001)

Phase diagram of the Hubbard model: Beyond the dynamical mean field

M. Jarrell[1], Th. Maier[2], M. H. Hettler[3] and A. N. Tahvildarzadeh[1]

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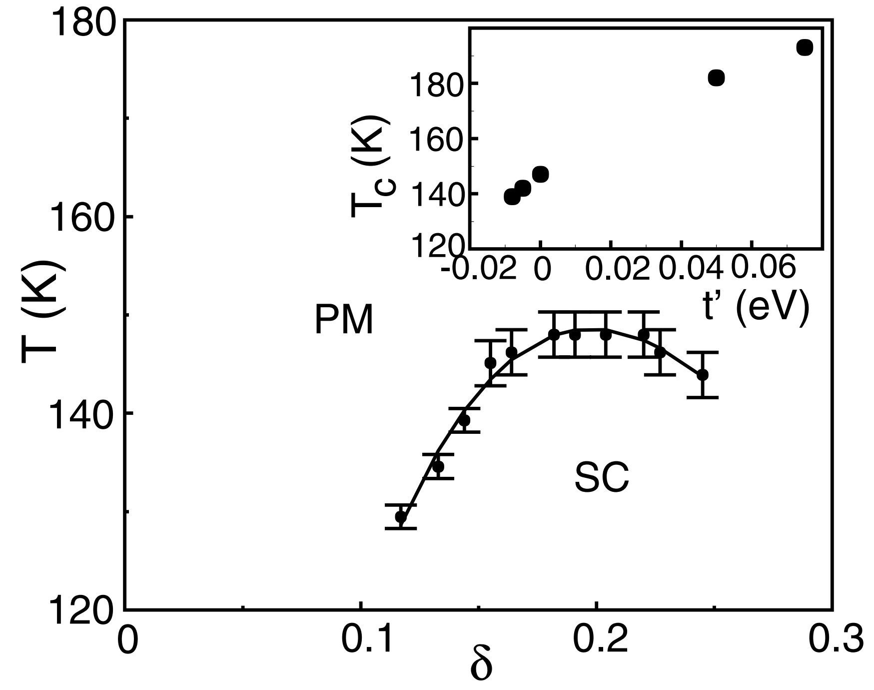

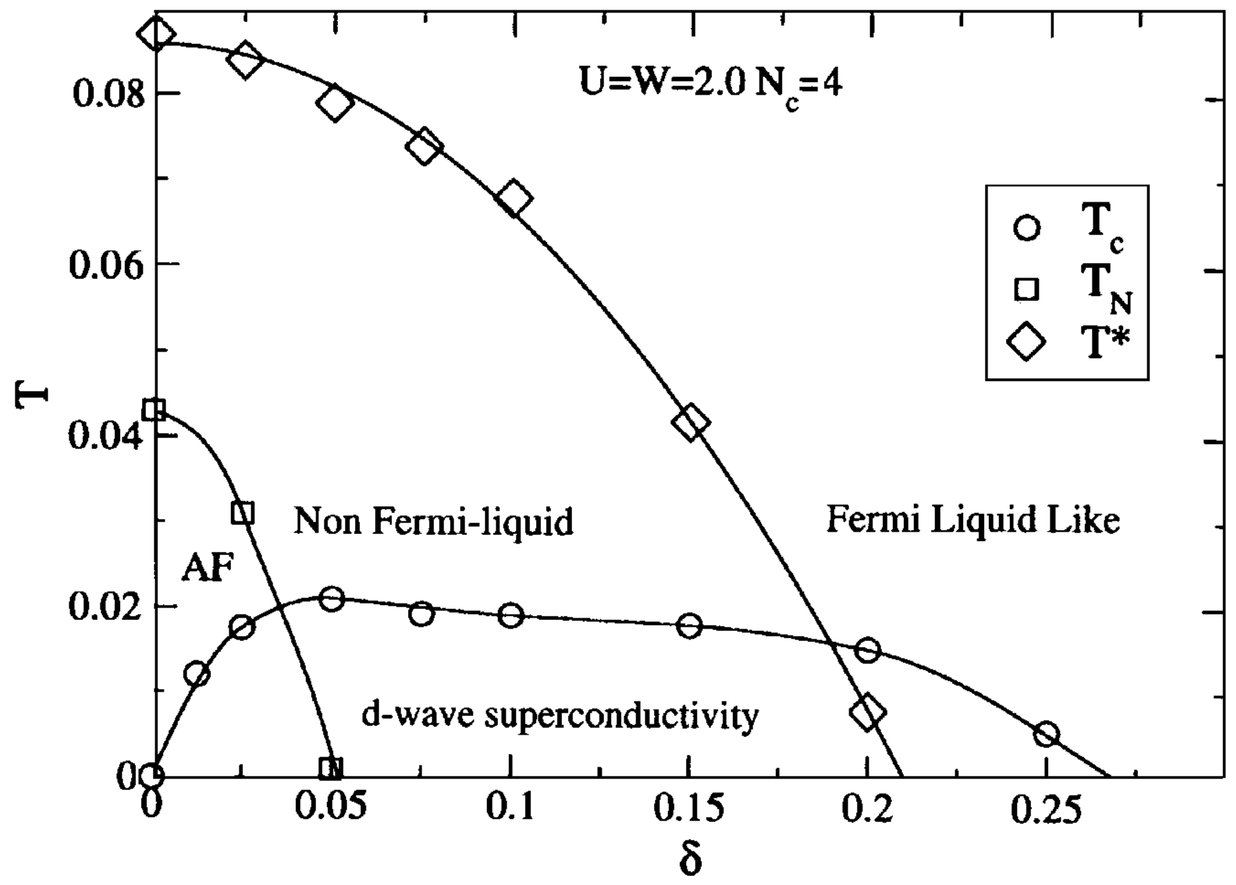

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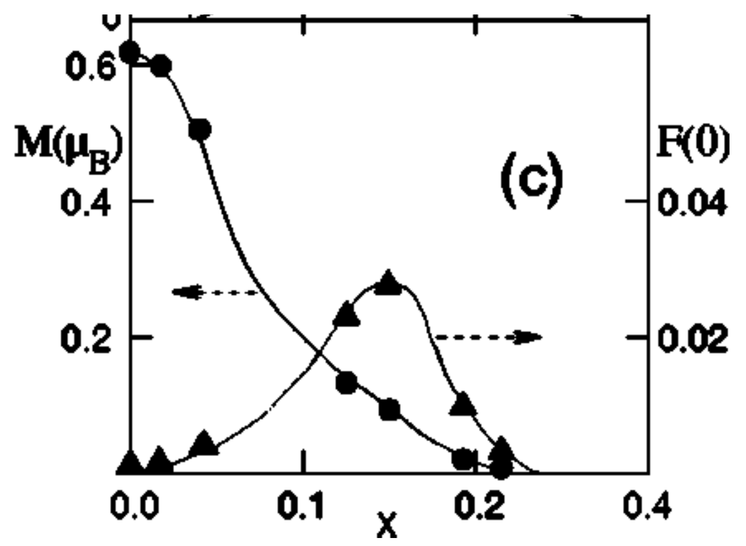

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PRL **95,** 237001 (2005) PHYSICAL REVIEW LETTERS week ending 2 DECEMBER 2005

Systematic Study of *d*-Wave Superconductivity in the 2D Repulsive Hubbard Model

T. A. Maier,[1] M. Jarrell,[2] T. C. Schulthess,[1] P. R. C. Kent,[3] and J. B. White[1]

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2005 DCA/QMC on up to 26-site clusters

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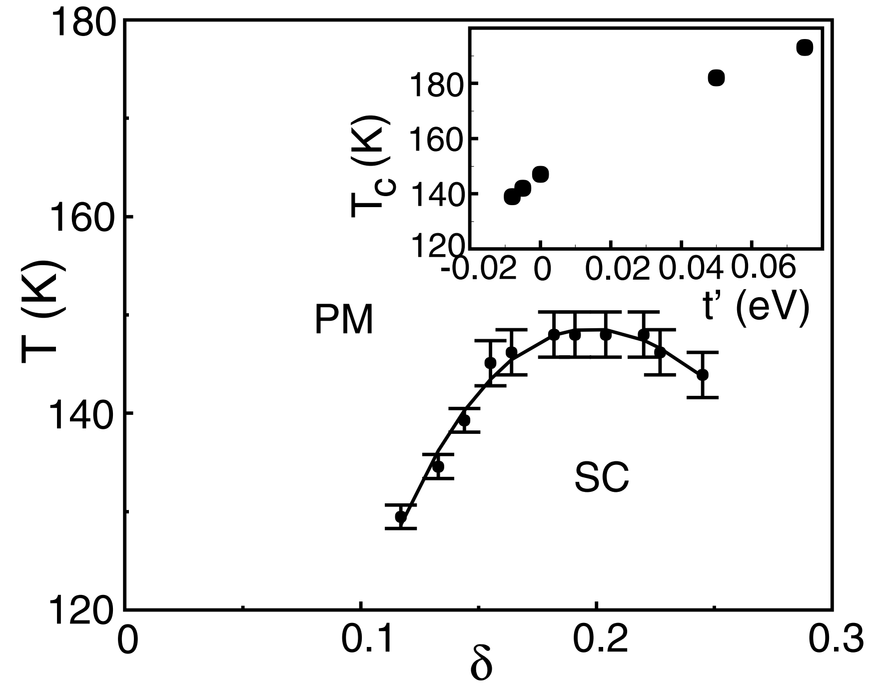

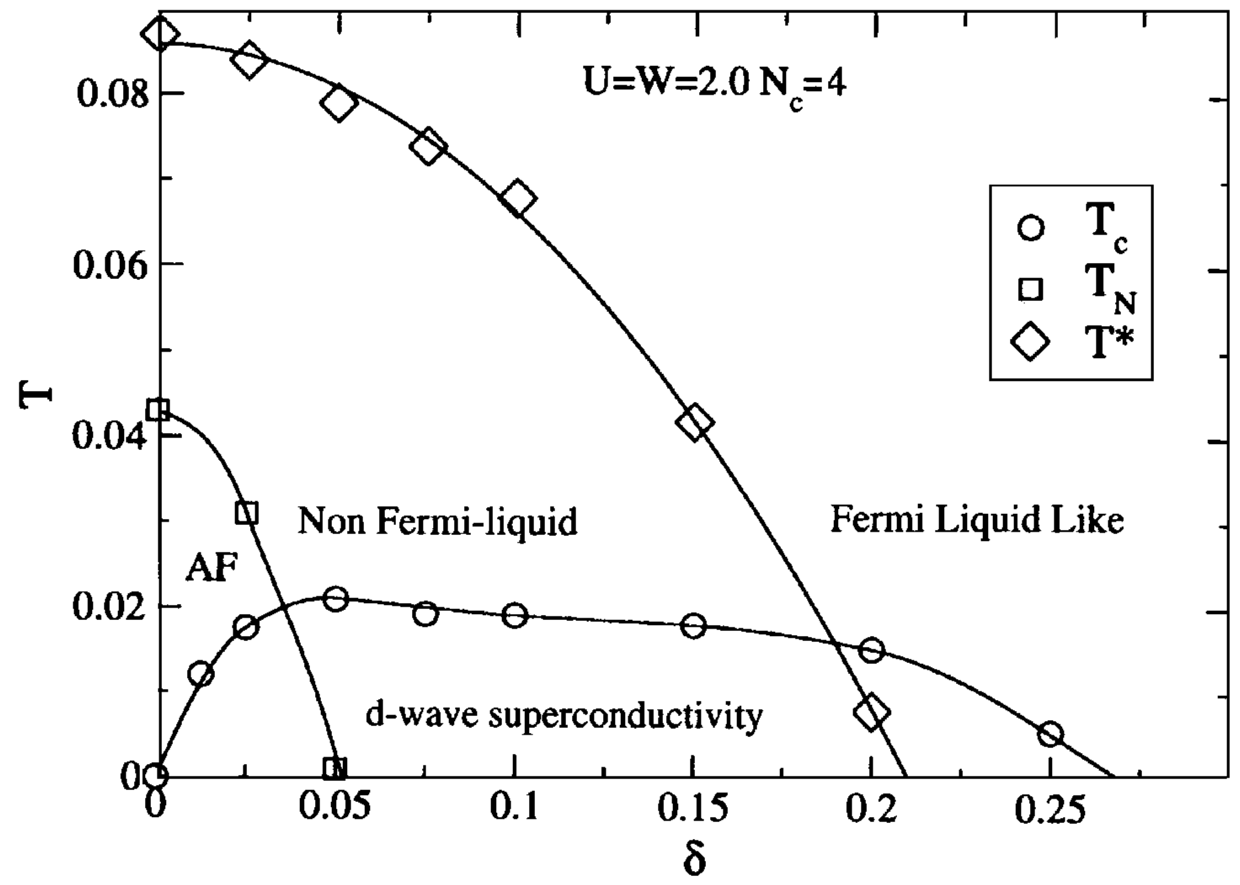

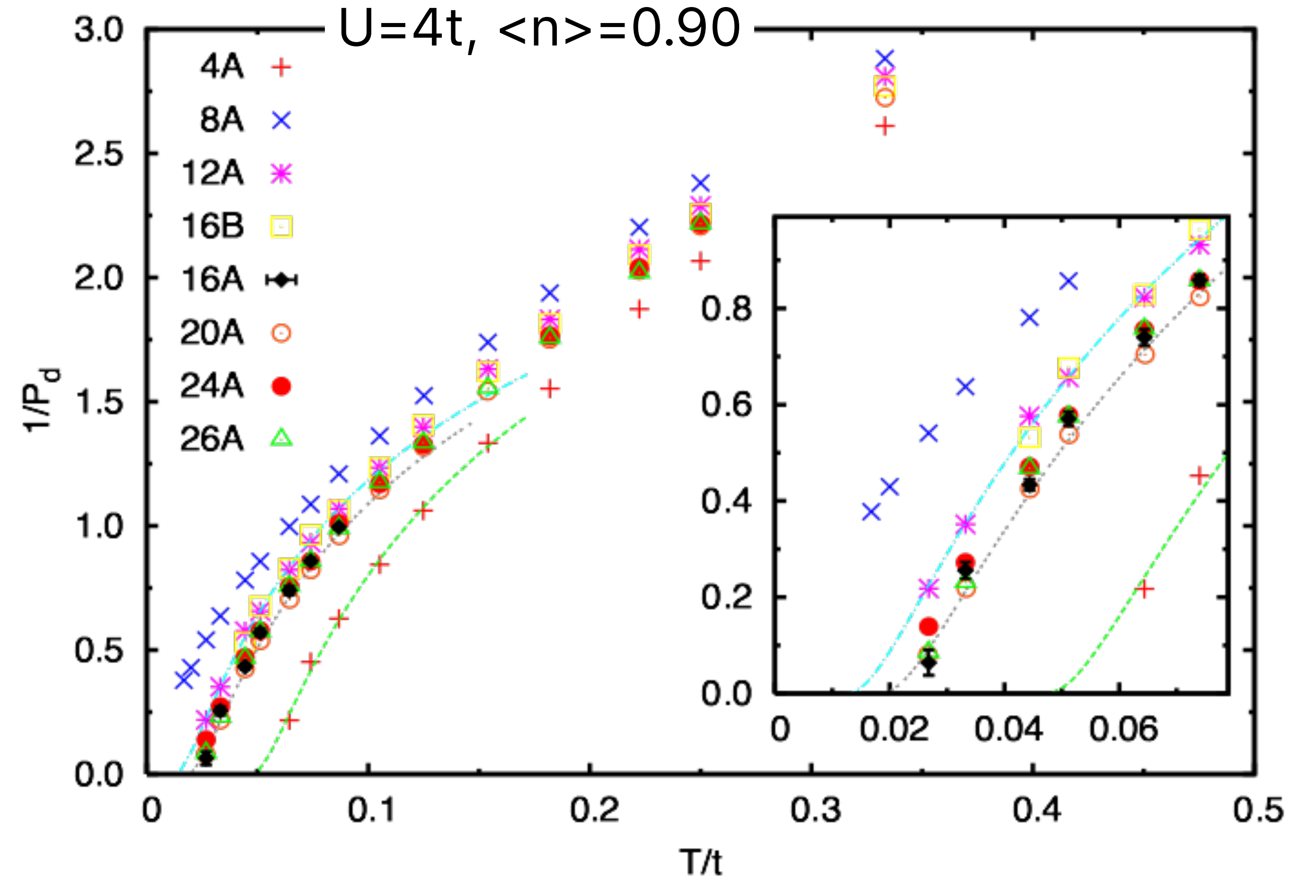

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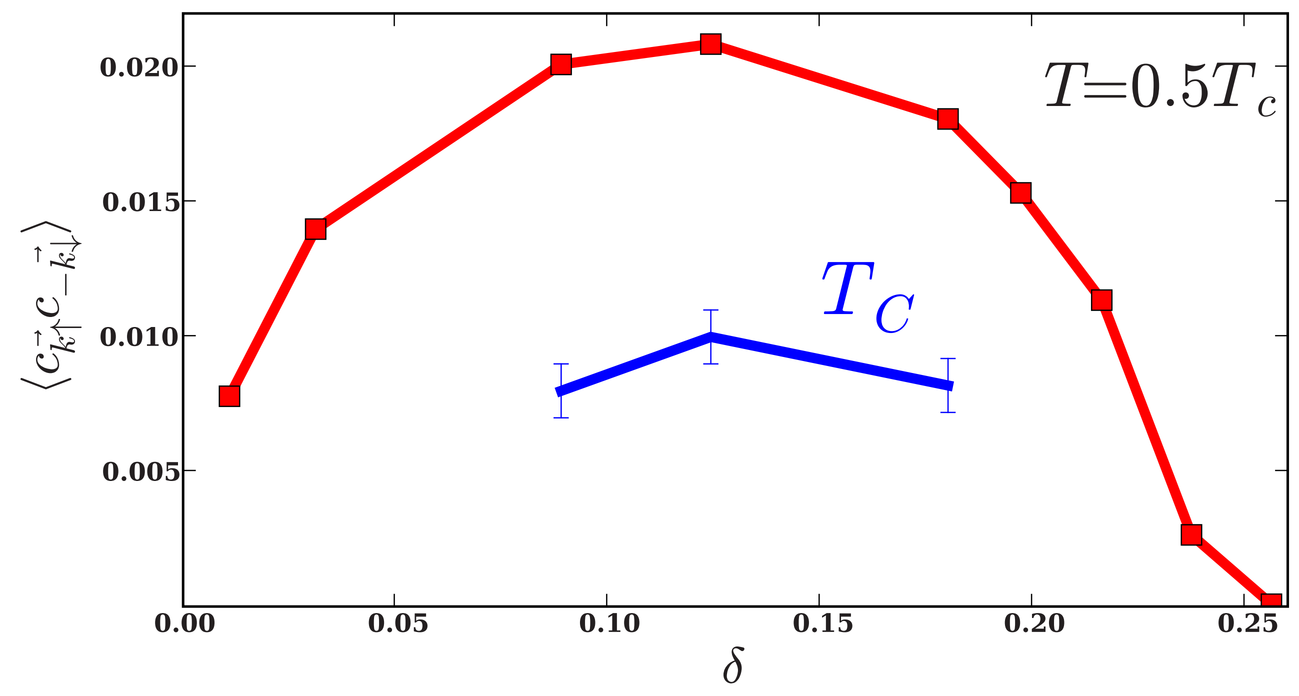
PHYSICAL REVIEW B **76**, 104509 (2007)

Strongly correlated superconductivity: A plaquette dynamical mean-field theory study

Kristjan Haule and Gabriel Kotliar



2007/8

Quantum cluster with ED/CT-HYB solver

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Anomalous superconductivity and its competition with antiferromagnetism in doped Mott insulators

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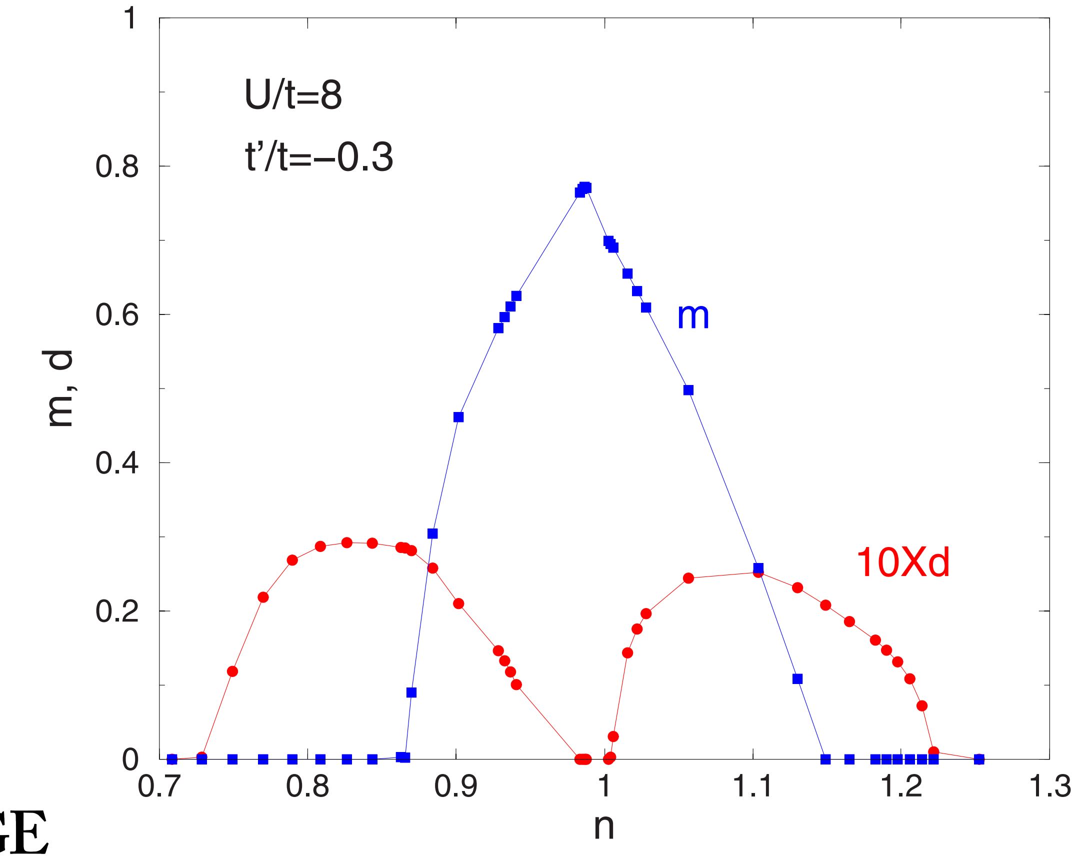

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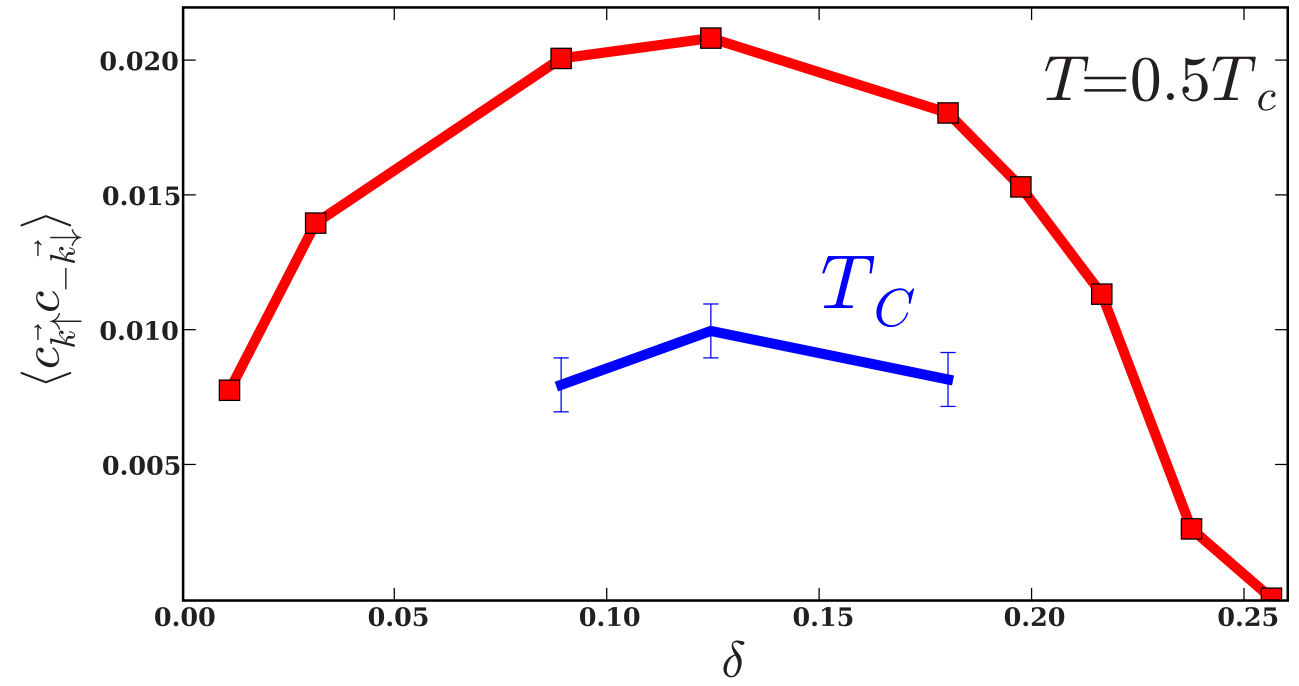

PRL **110**, 216405 (2013) PHYSICAL REVIEW LETTERS week ending 24 MAY 2013

Superconductivity and the Pseudogap in the Two-Dimensional Hubbard Model

Emanuel Gull,[1,2] Olivier Parcollet,[3] and Andrew J. Millis[4]

2007/8

Quantum cluster with
ED/CT-HYB solver

2013

DCA in
superconducting phase

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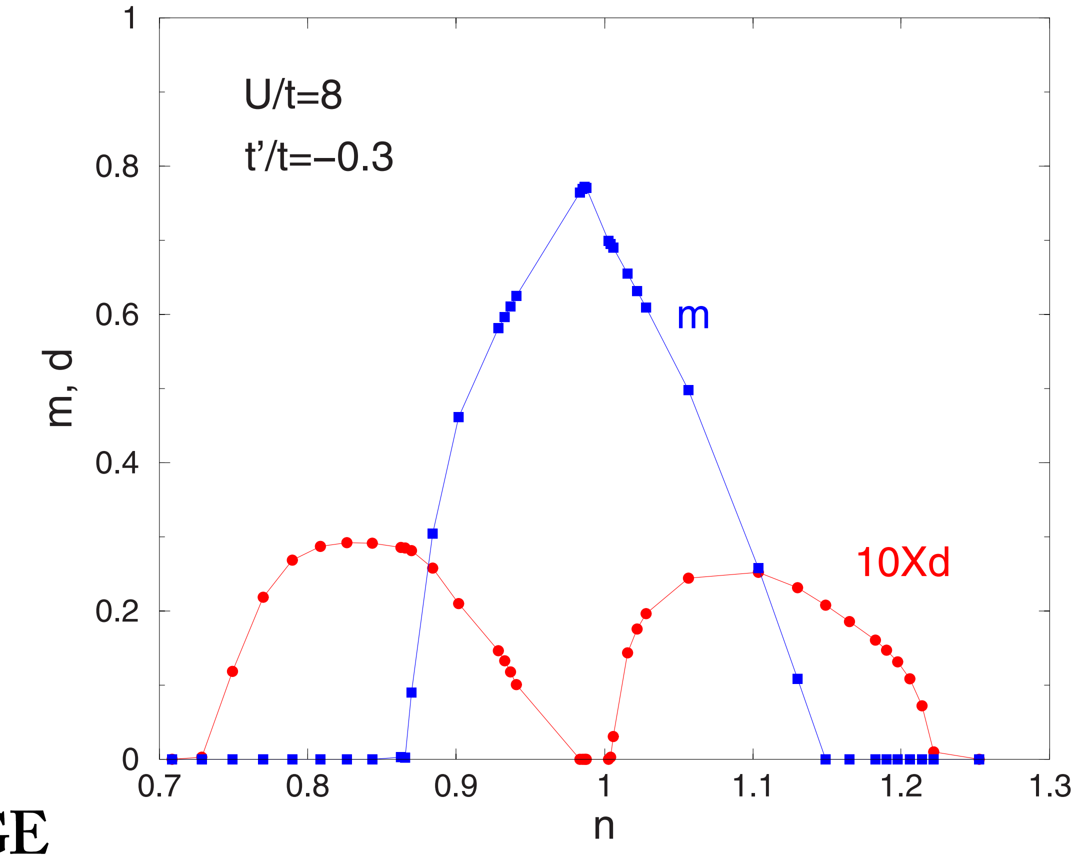

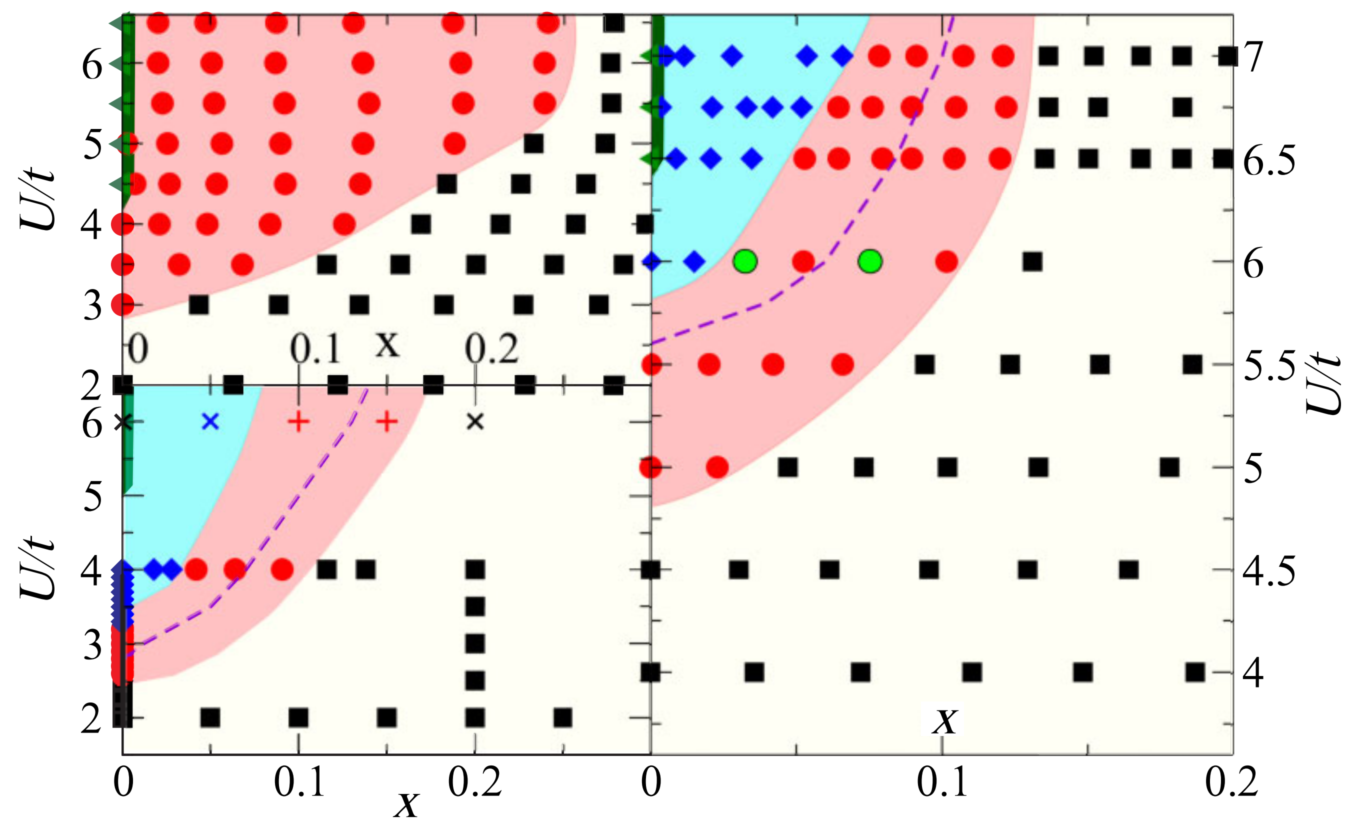

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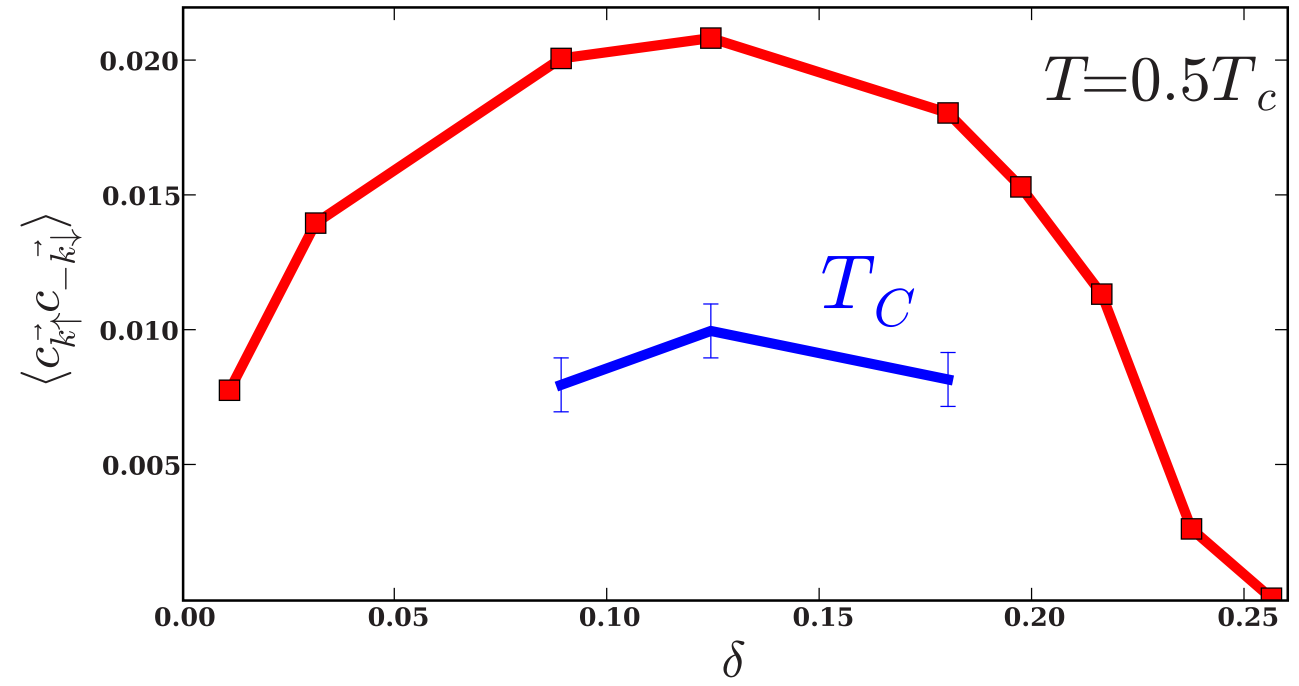

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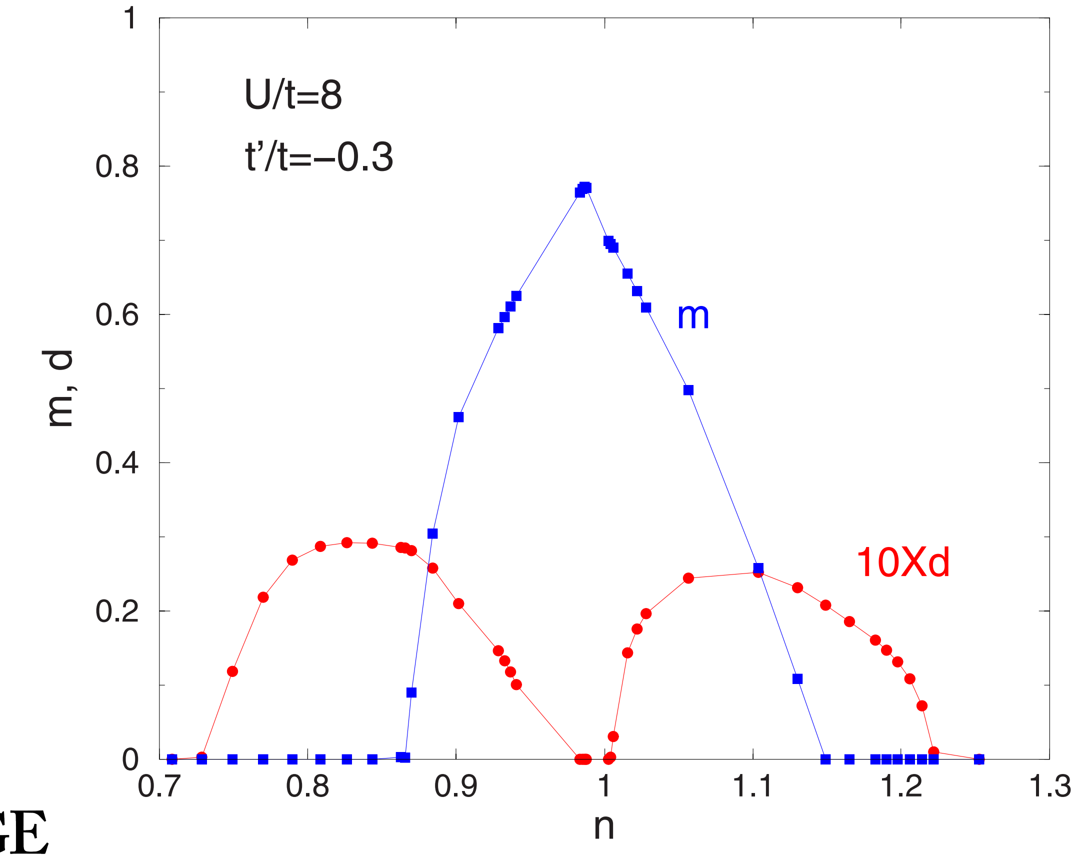


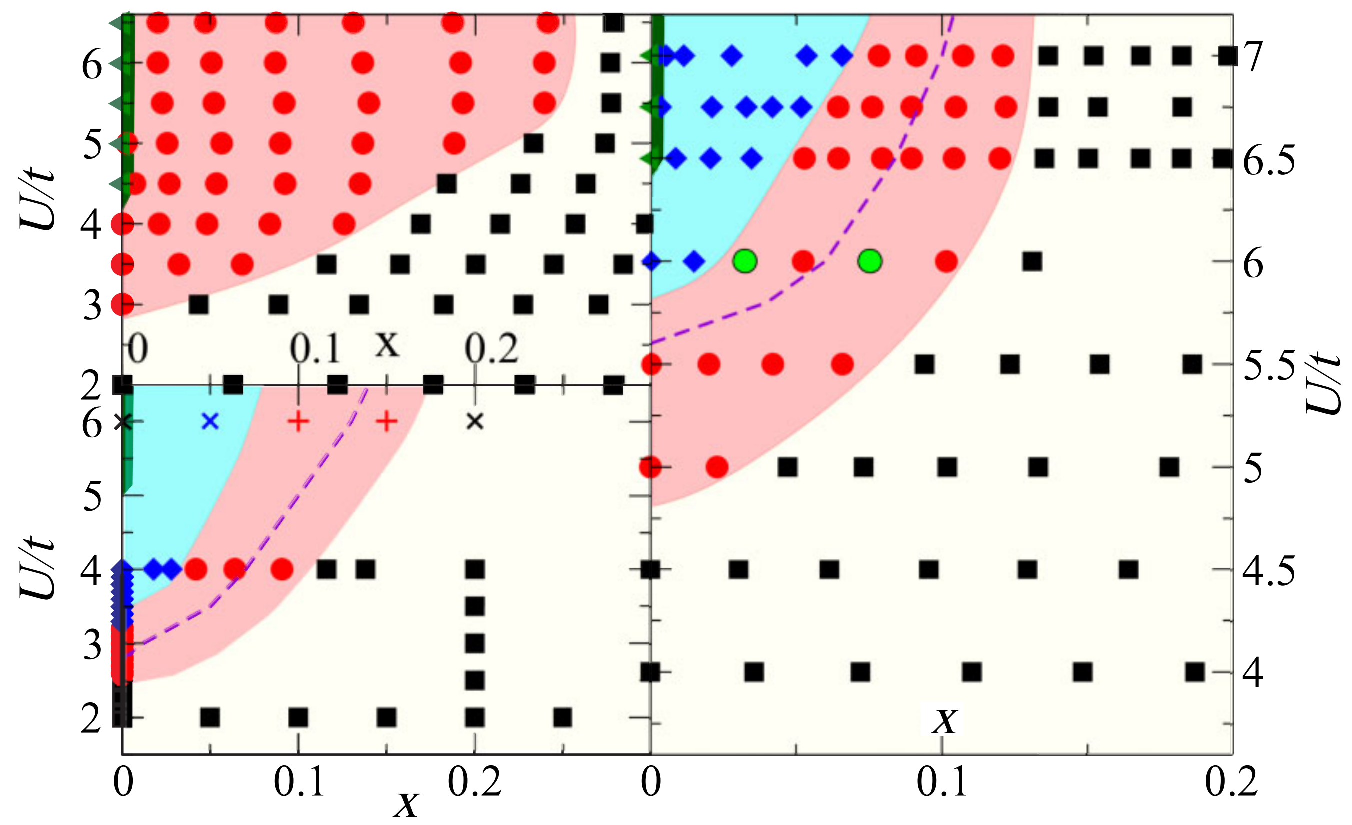
PRL **110**, 216405 (2013) PHYSICAL REVIEW LETTERS week ending 24 MAY 2013

Superconductivity and the Pseudogap in the Two-Dimensional Hubbard Model

Emanuel Gull,[1,2] Olivier Parcollet,[3] and Andrew J. Millis[4]

2013

DCA in superconducting phase



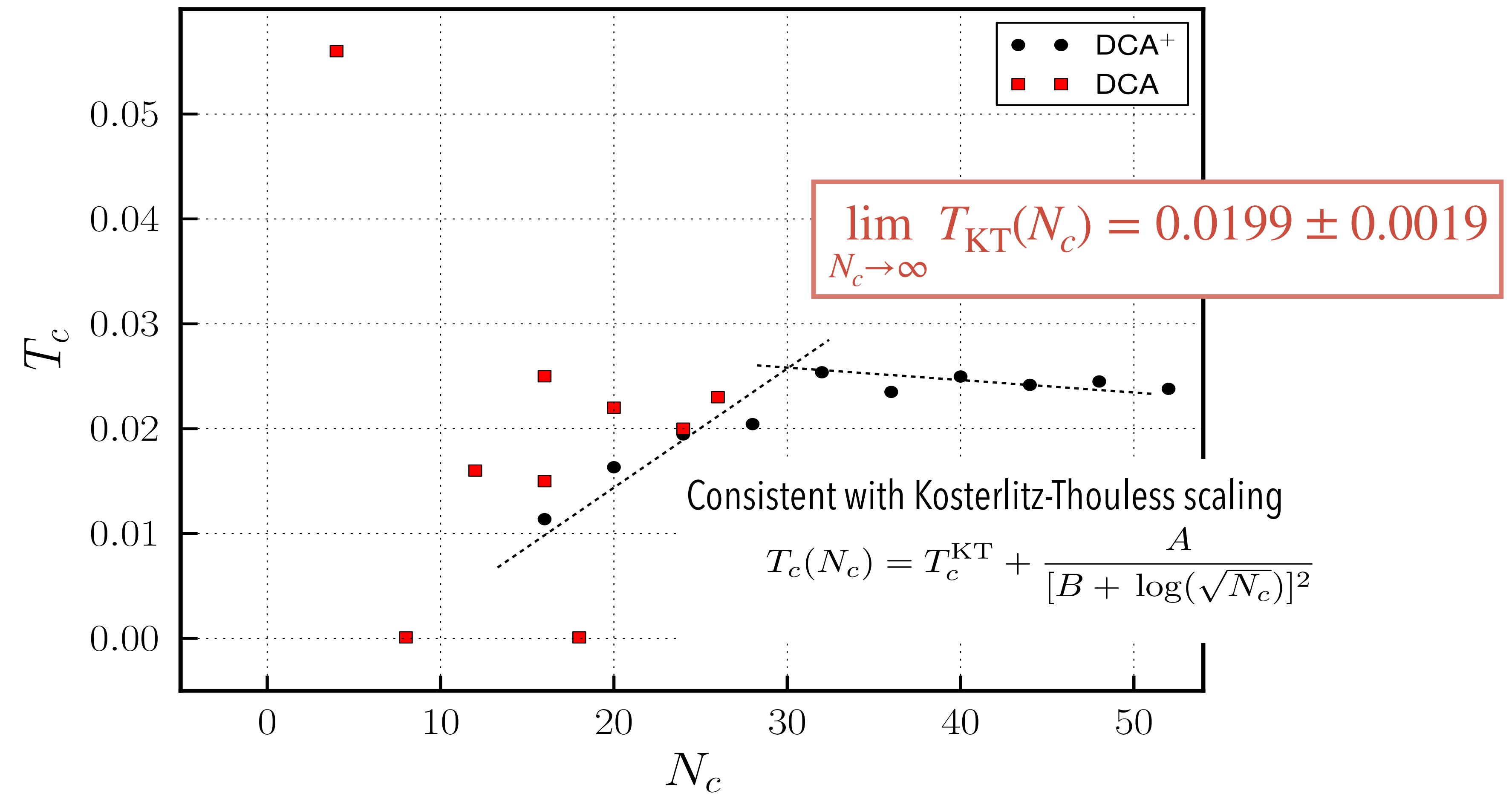
PHYSICAL REVIEW B **89**, 195133 (2014)

Two-particle correlations in a dynamic cluster approximation with continuous momentum dependence: Superconductivity in the two-dimensional Hubbard model

Peter Staar,[1] Thomas Maier,[2,3] and Thomas C. Schulthess[1,2,4]

2014

DCA on clusters up to 56 sites



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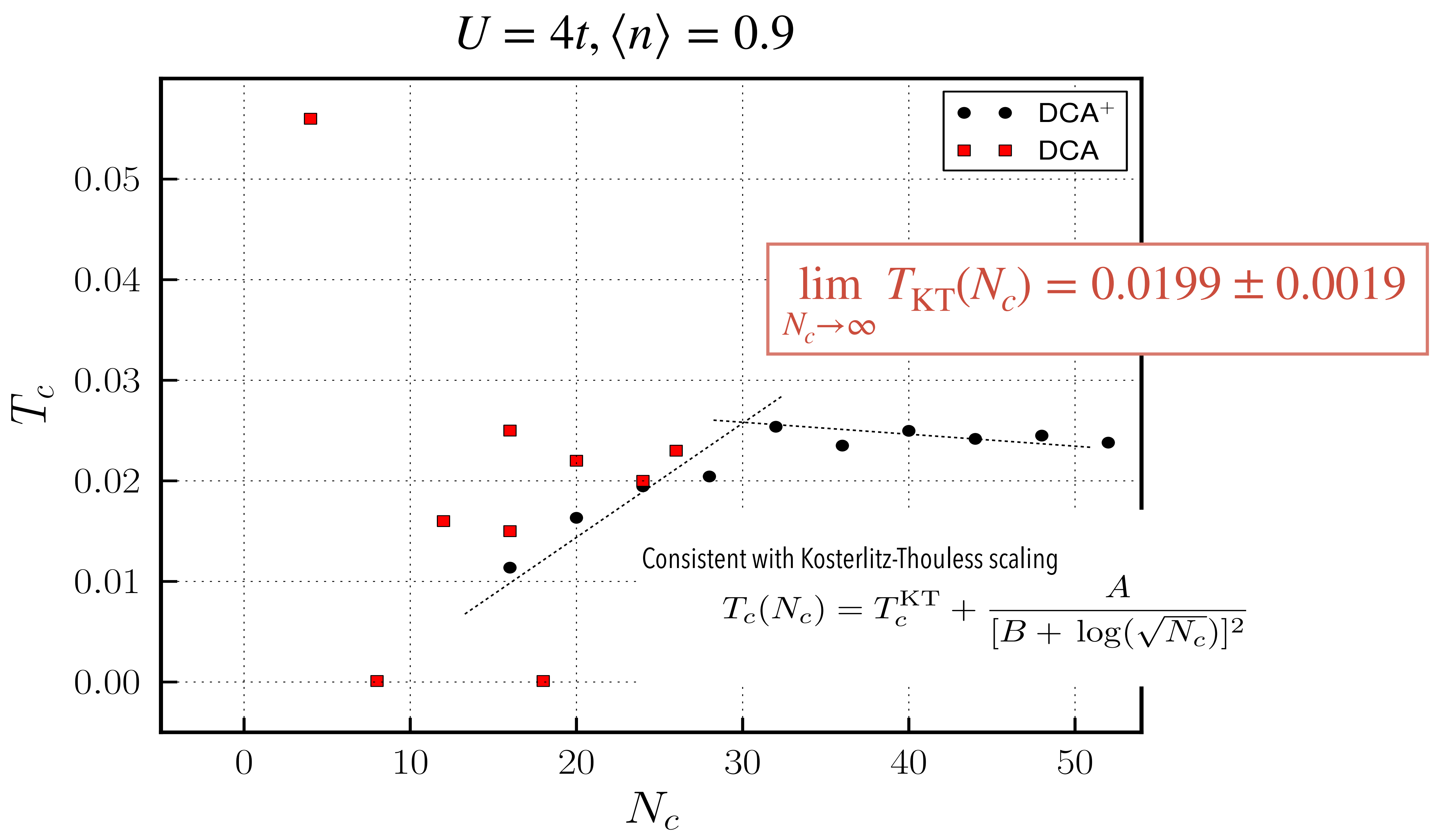
Larger U



- **Highest T_c for U ~ W=8t**

Staar *et al.*, PRB '14

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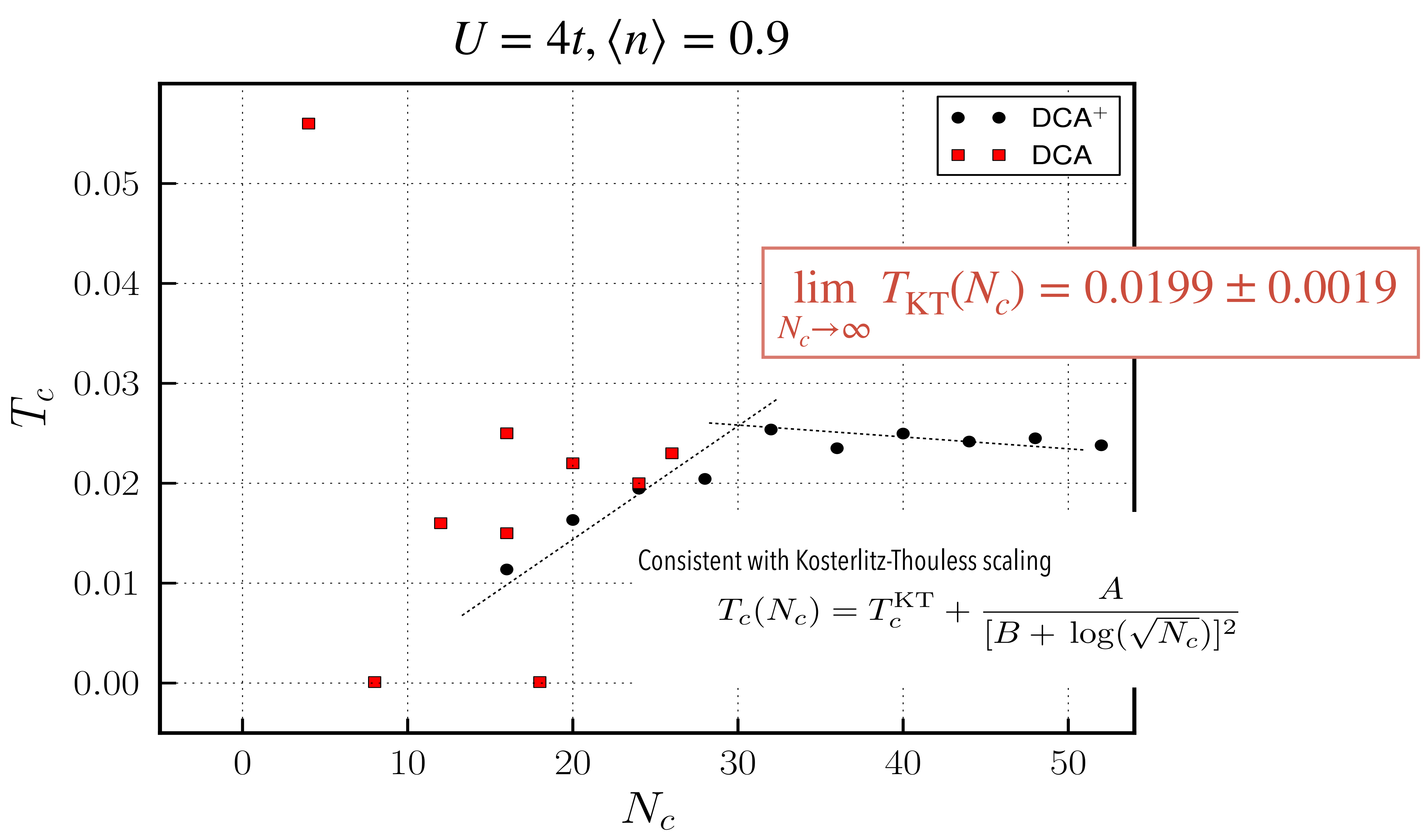

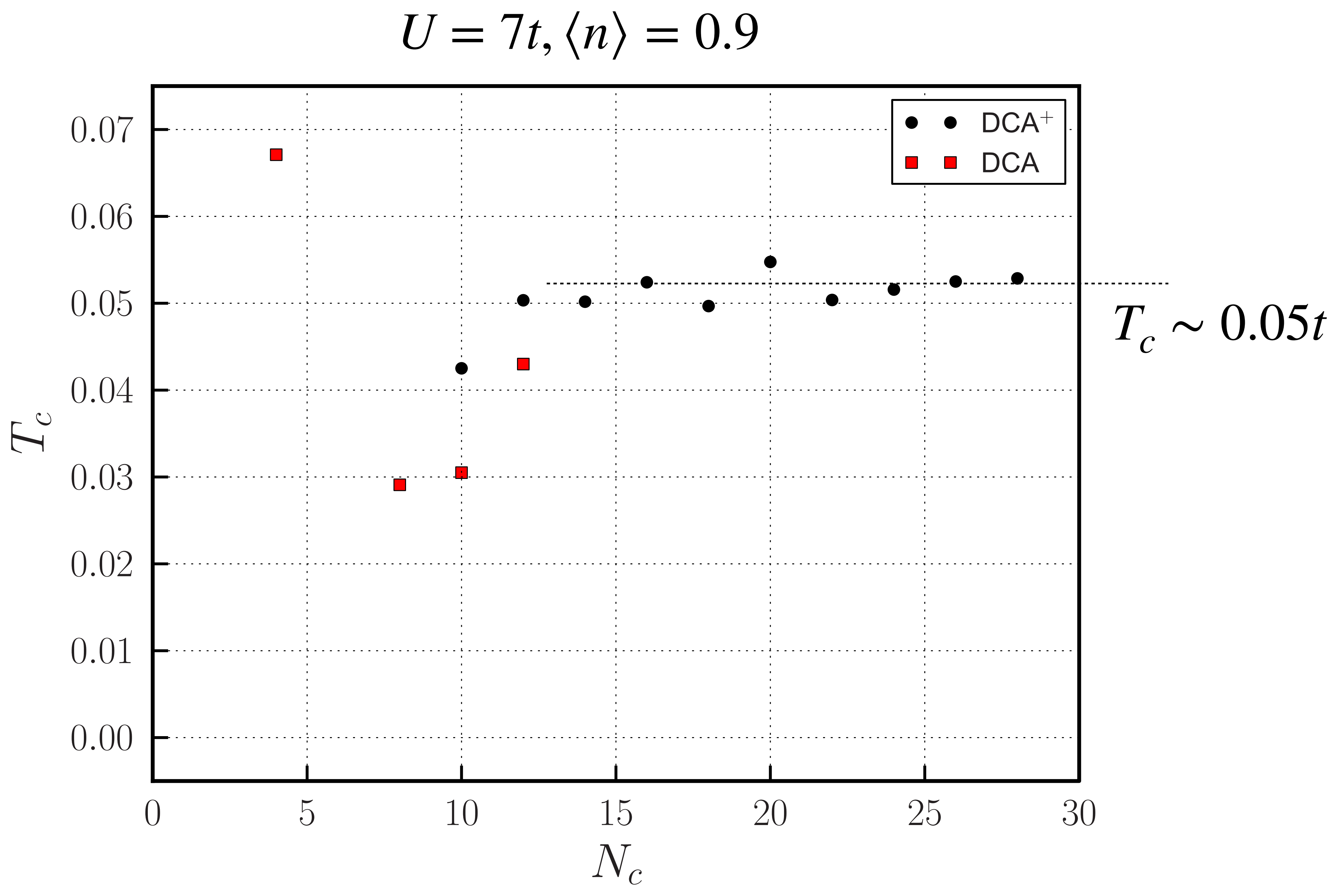

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Staar *et al.*, PRB '14

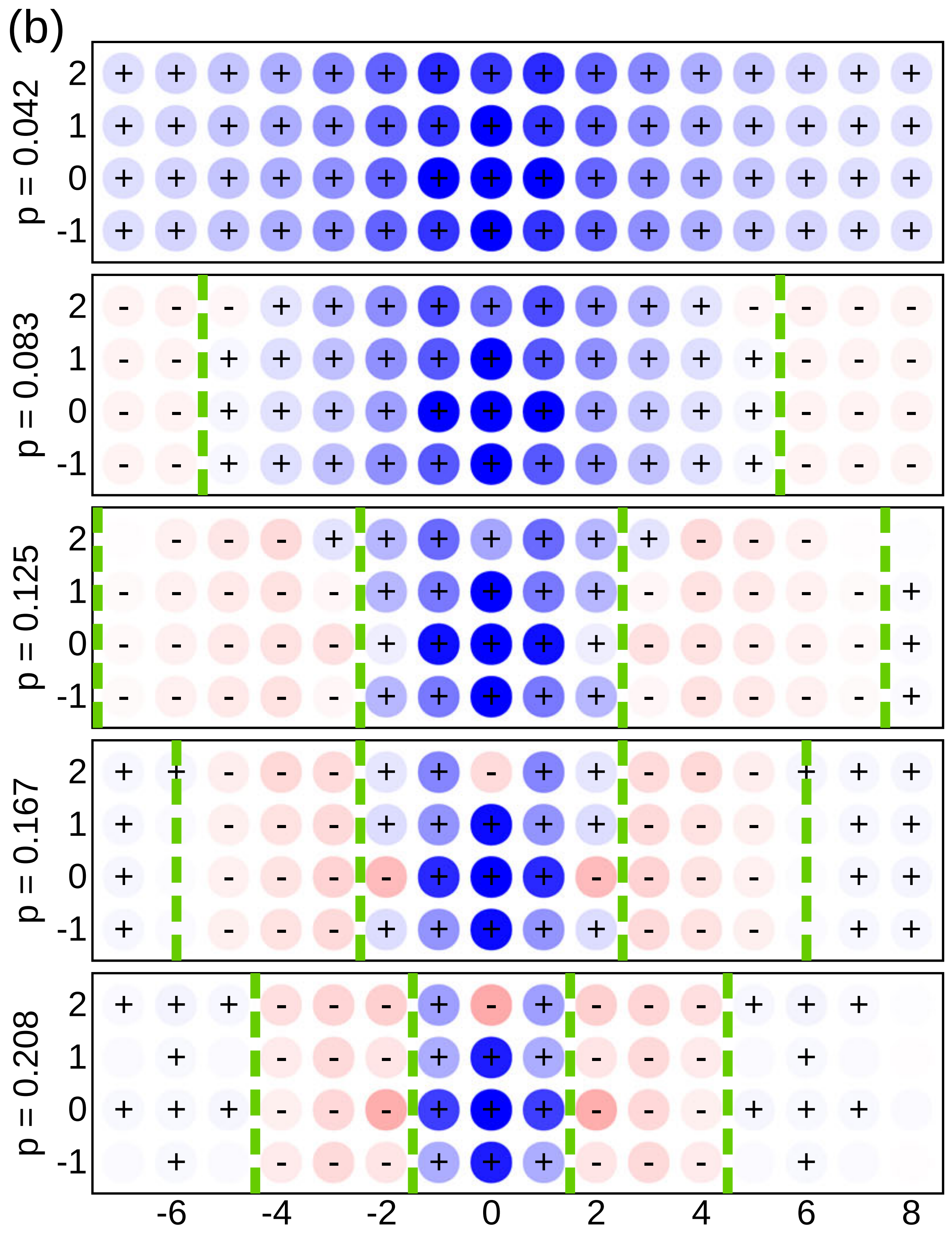
Stripes?

npj | Quantum Materials 2018

ARTICLE OPEN

Stripe order from the perspective of the Hubbard model

Edwin W. Huang[1,2], Christian B. Mendl[2], Hong-Chen Jiang[2], Brian Moritz[2,3] and Thomas P. Devereaux[2,4]



DQMC on 16 x 4 Hubbard:

$U/t = 6, t'/t = -0.25, T/t = 0.22$

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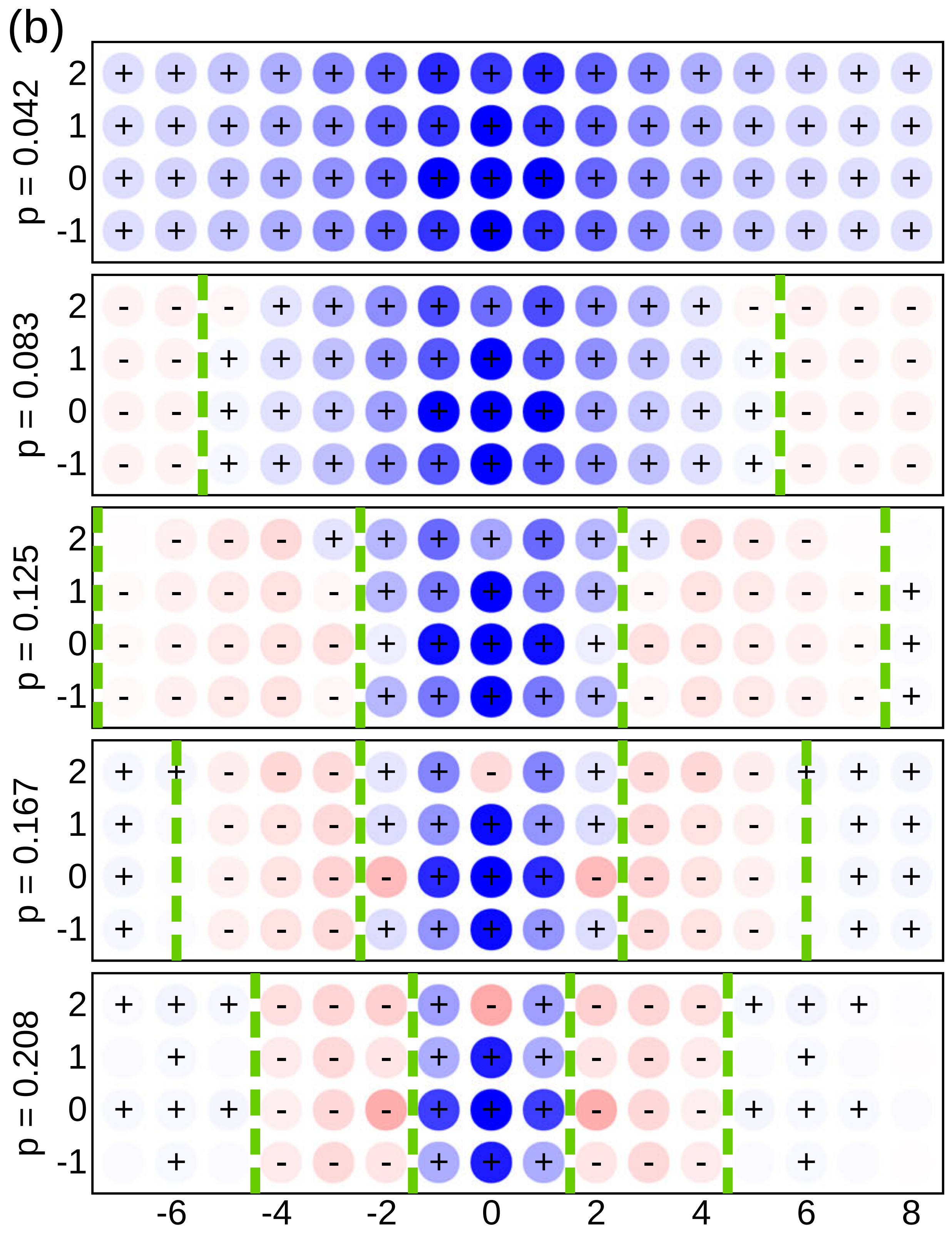

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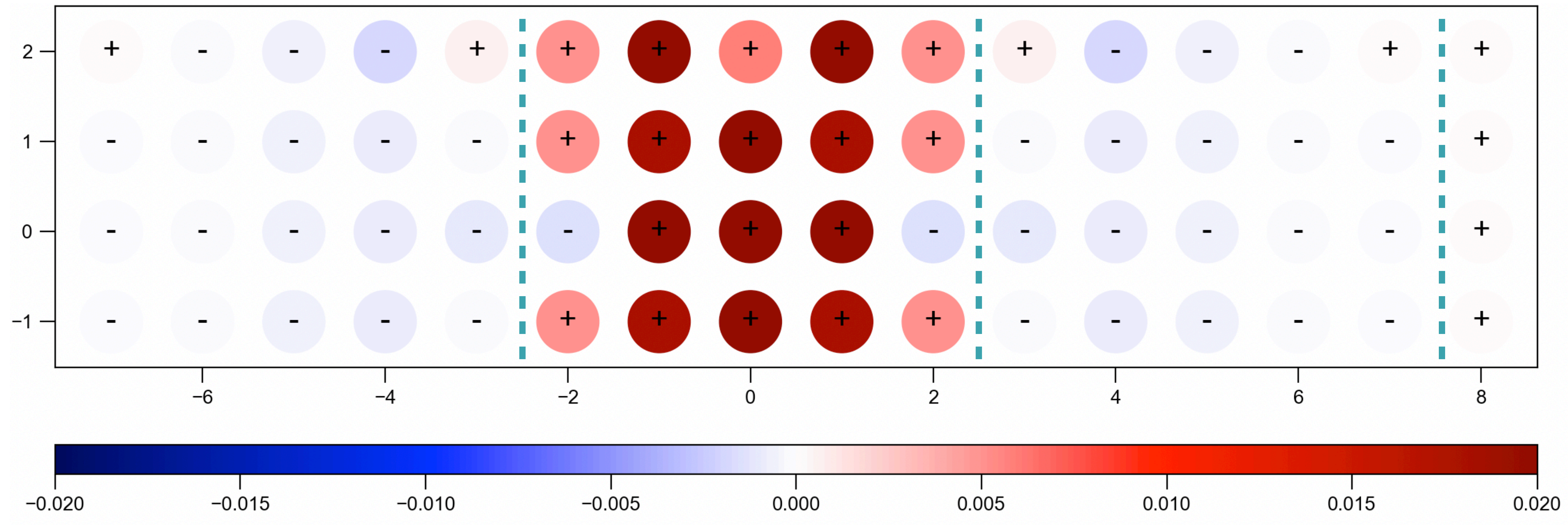
CT-AUX on finite size 16 x 4 cluster
$U/t = 5, t'/t = -0.25, T/t = 0.22$



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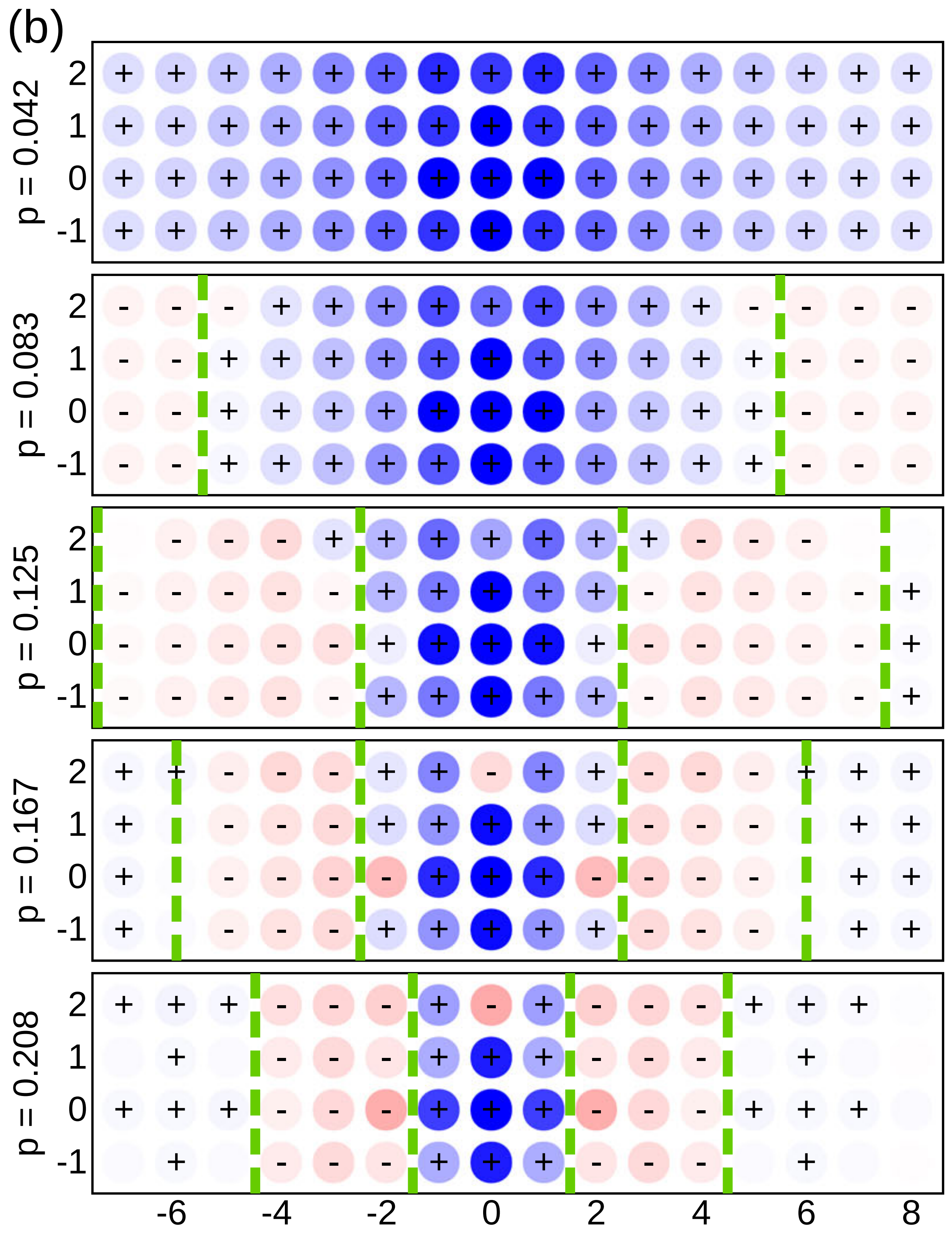

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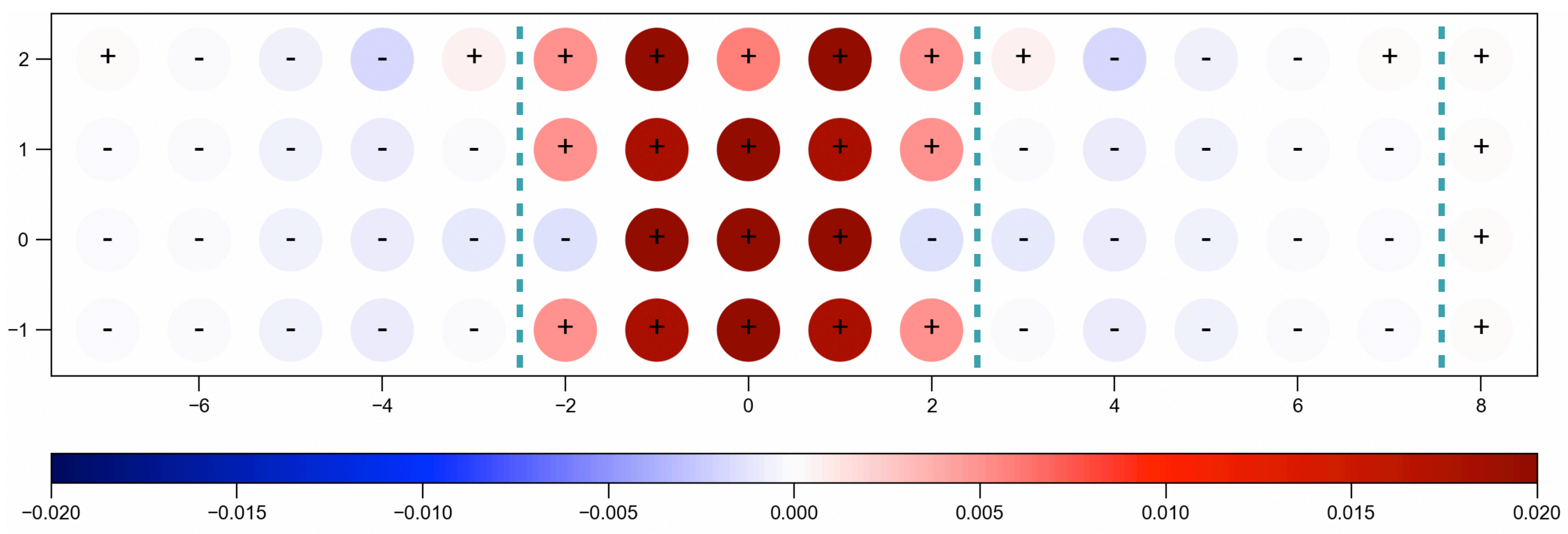
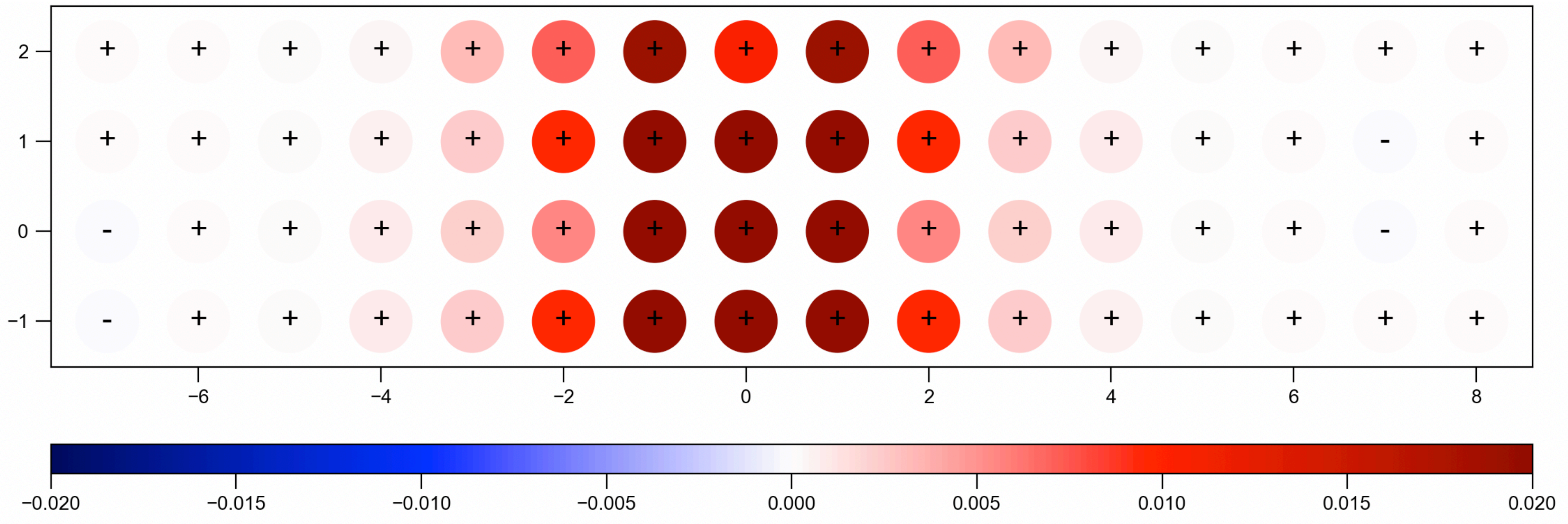


DCA/CT-AUX (with mean-field)

$U/t = 5, t'/t = -0.25, T/t = 0.17$



Stripes?

npj Quantum Materials 2018

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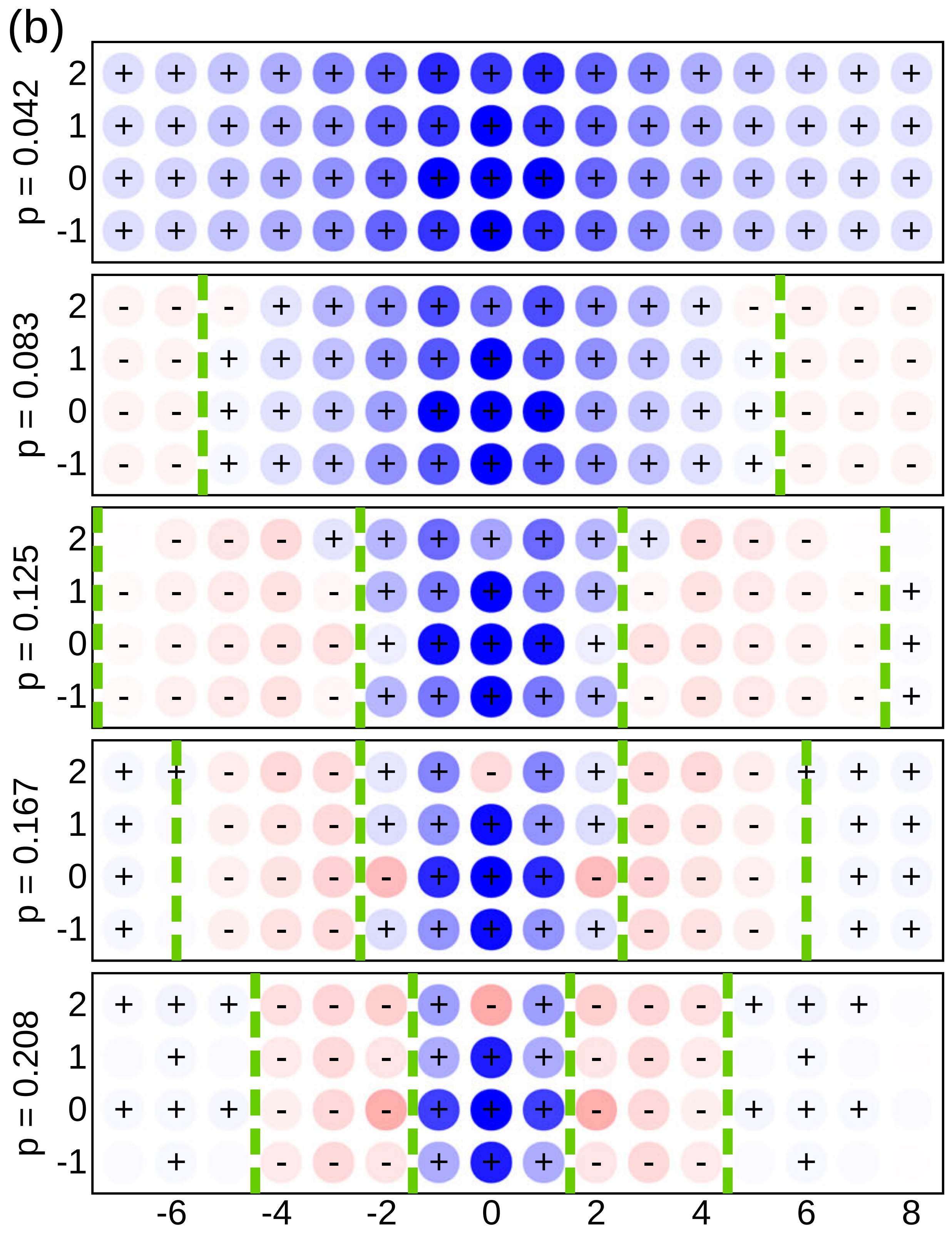

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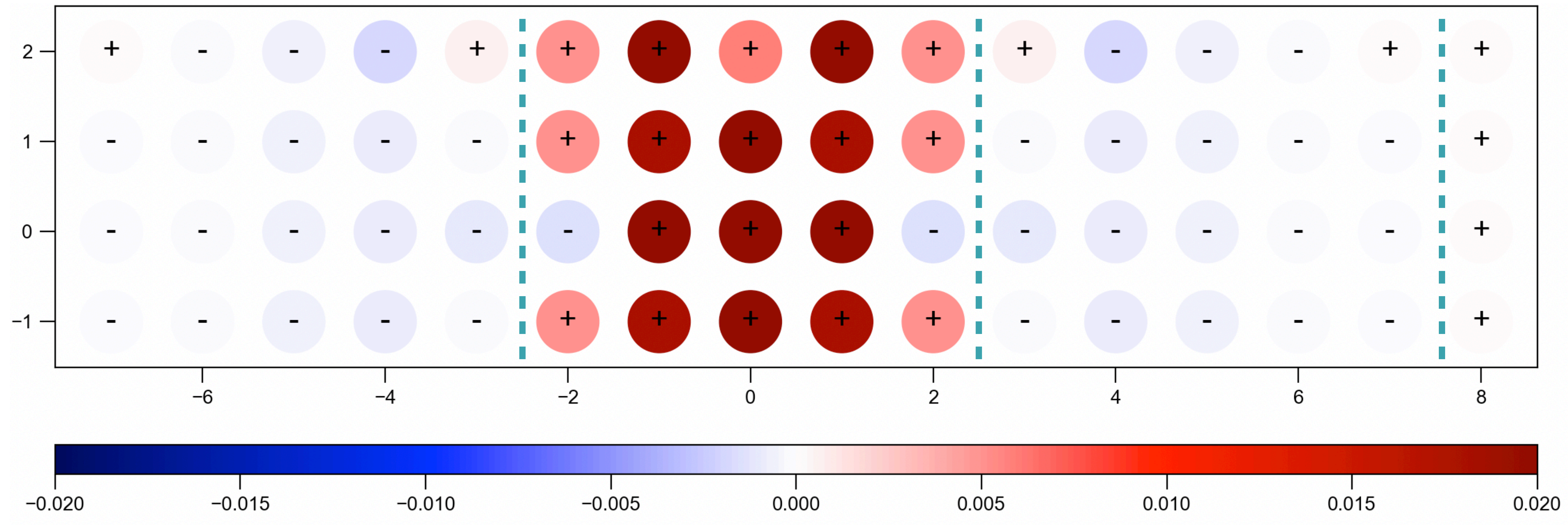

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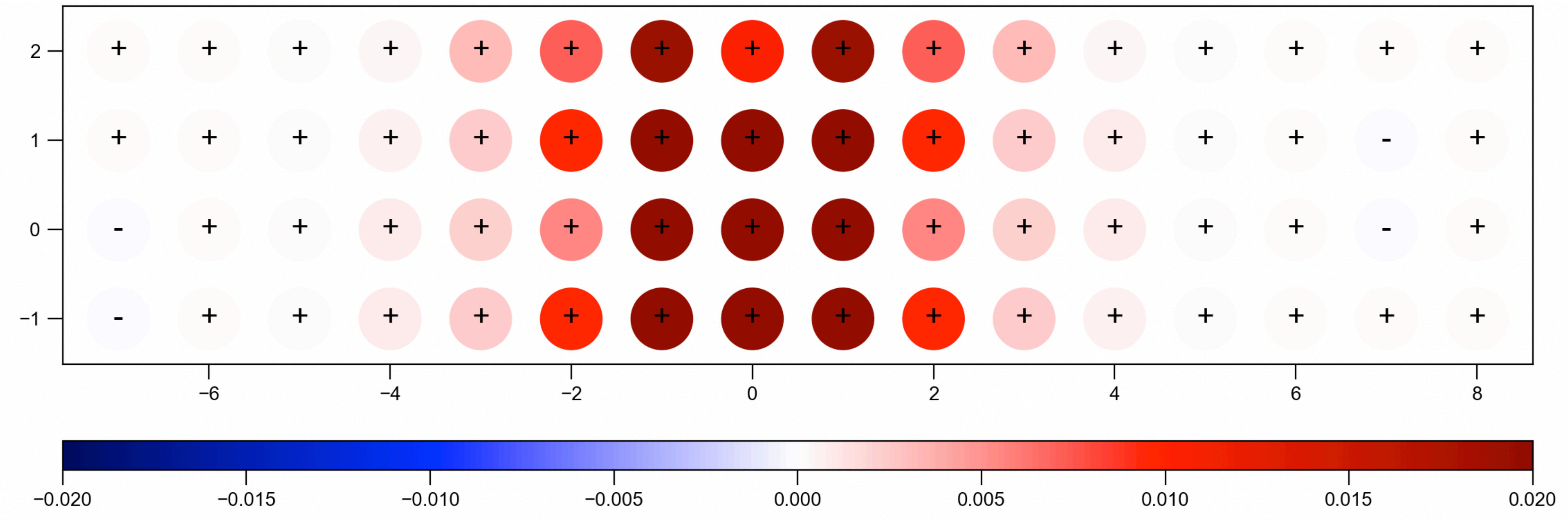
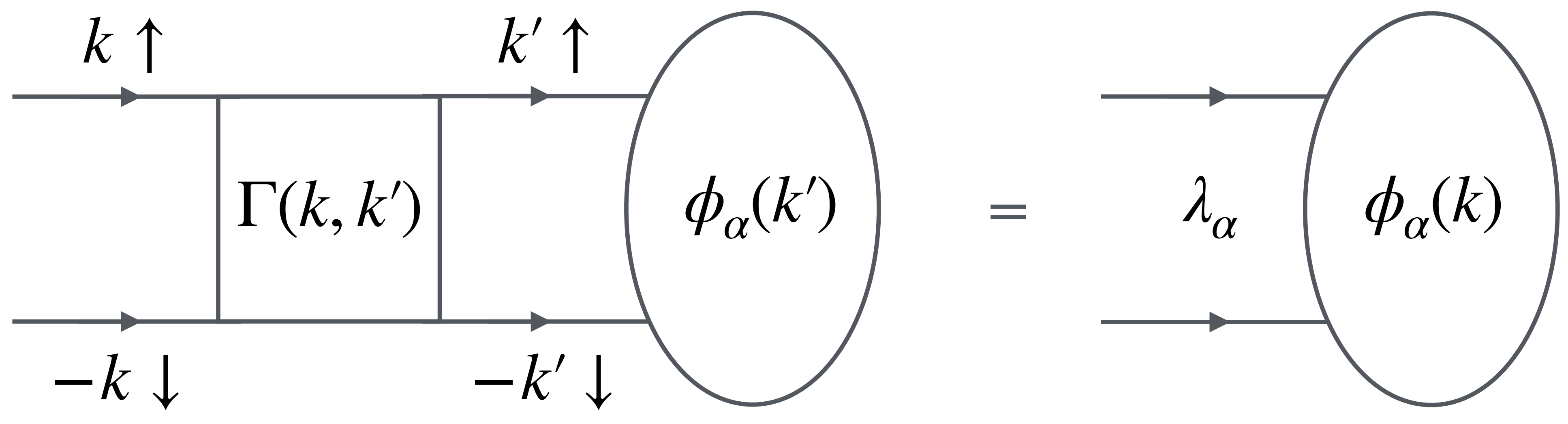


- **Mean-field coupling frustrates stripe formation and favors superconductivity**

Pairing interaction and Bethe-Salpeter equation

Particle-particle Bethe-Salpeter equation relates gap function $\phi(k)$ to pairing interaction $\Gamma(k, k')$



$$-\frac{T}{N}\sum_{k'} \Gamma(k, k')G(k')G(-k')\phi_\alpha(k') = \lambda_\alpha \phi_\alpha(k)$$

BCS: $$-\frac{1}{N}\sum_{k'} \frac{V_{kk'}\Delta_{k'}\tanh(\frac{1}{2}\beta E_{k'})}{2E_{k'}} = \Delta_k$$

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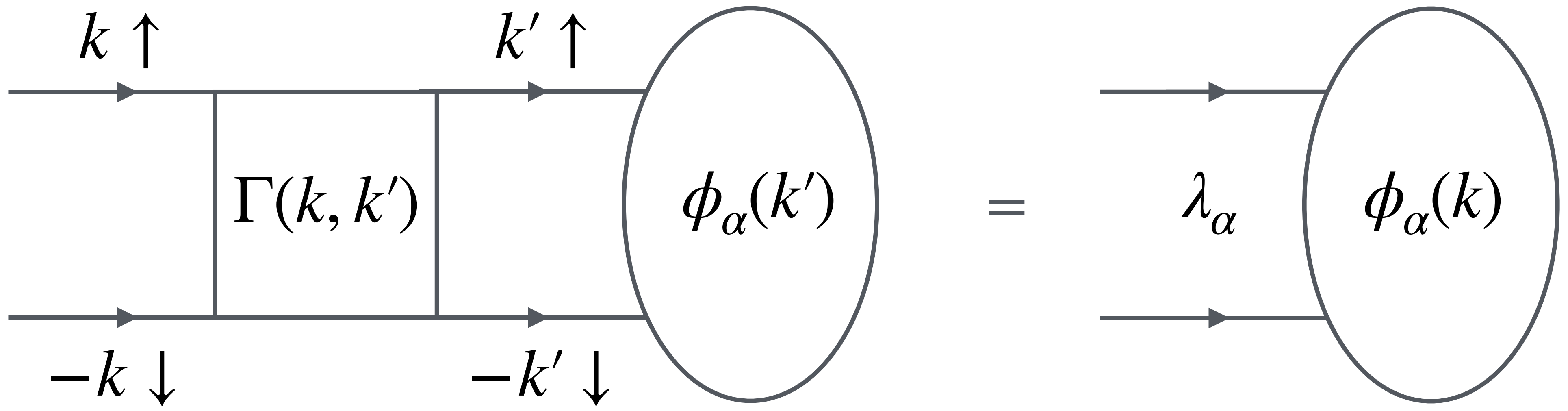

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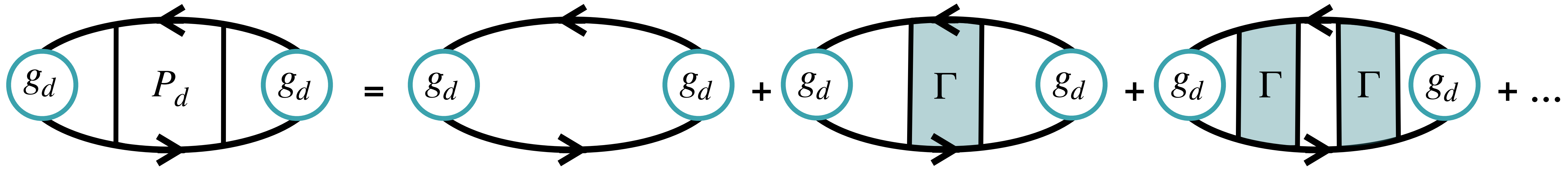
d-wave pair-field susceptibility

$$P_d = \int_0^\beta d\tau\langle\mathcal{T}_\tau\Delta(\tau)\Delta^\dagger(0)\rangle$$

$$\Delta^\dagger = \frac{1}{\sqrt{N}}\sum_k g_d(k)c^\dagger_{k\uparrow}c^\dagger_{-k\downarrow}$$



$$P_d(T) \sim \frac{1}{1-\lambda_d(T)}$$

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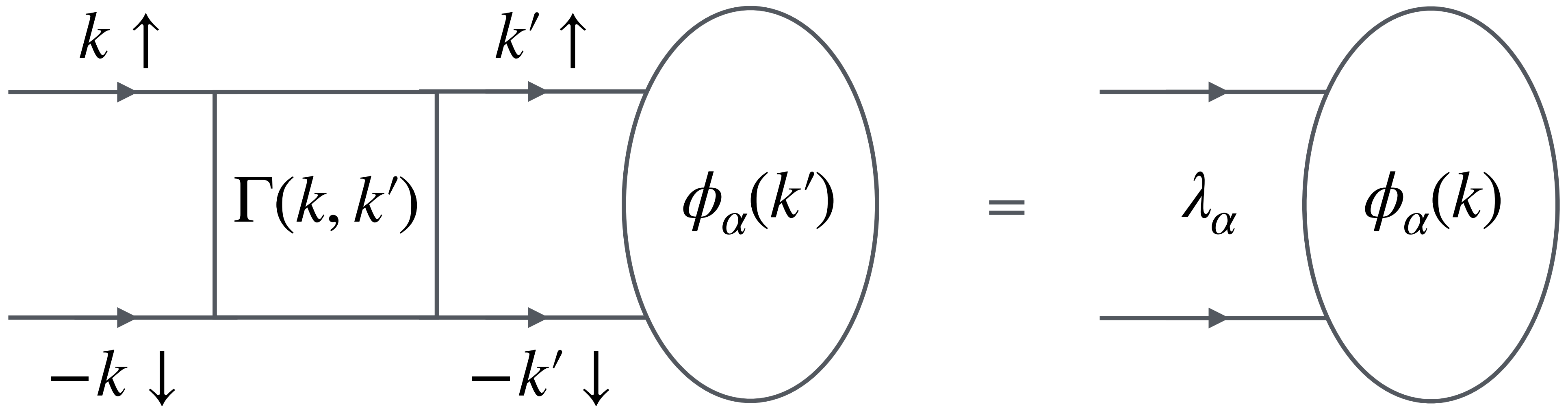

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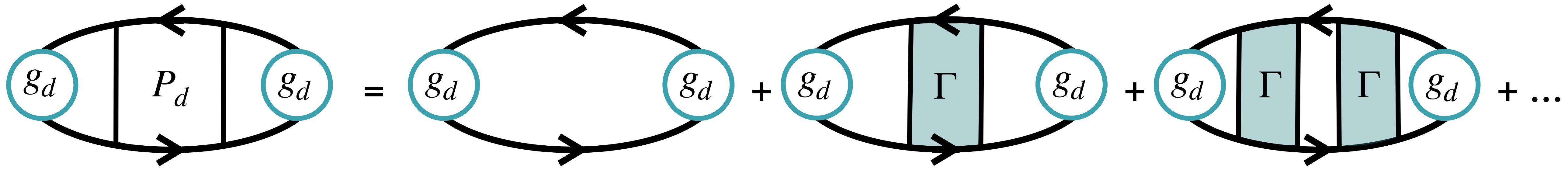


$$P_d(T) \sim \frac{1}{1-\lambda_d(T)}$$

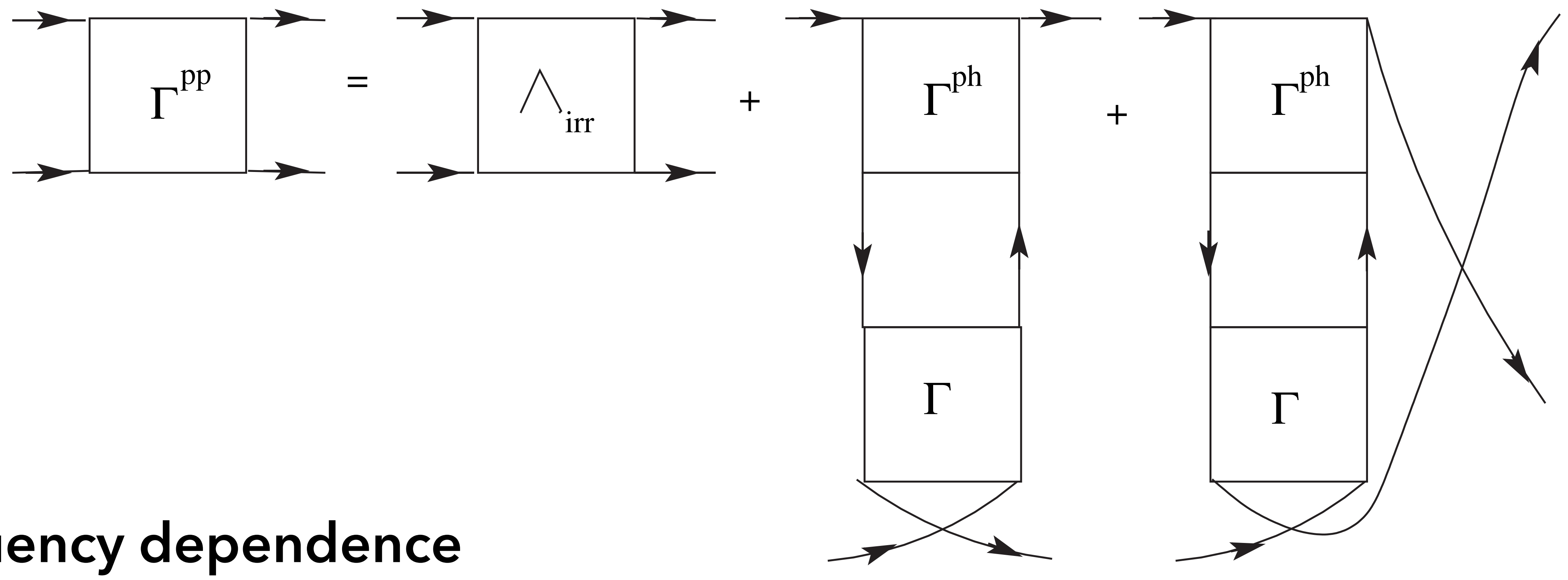
Separable approximation

$$\lambda_d(T) \approx V_d(T)P_{d,0}(T)$$

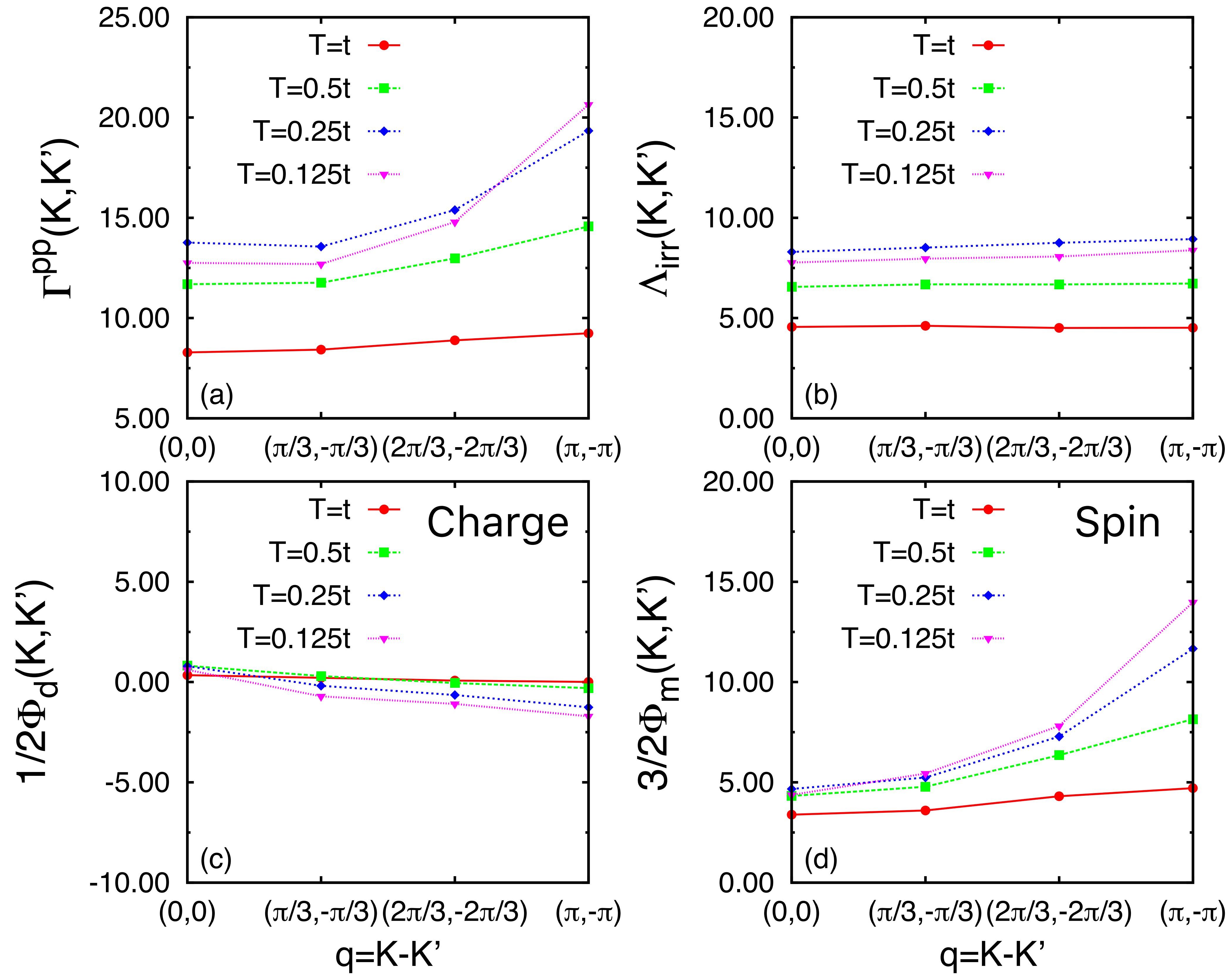
$$V_d = -\langle \phi_d | \Gamma | \phi_d \rangle\,;\; P_{d,0} = \frac{T}{N}\langle \phi_d | GG | \phi_d \rangle$$

BCS: $V_d(T) \approx \text{const.}\,;\; P_{d,0}(T) \sim \log(t/T)$

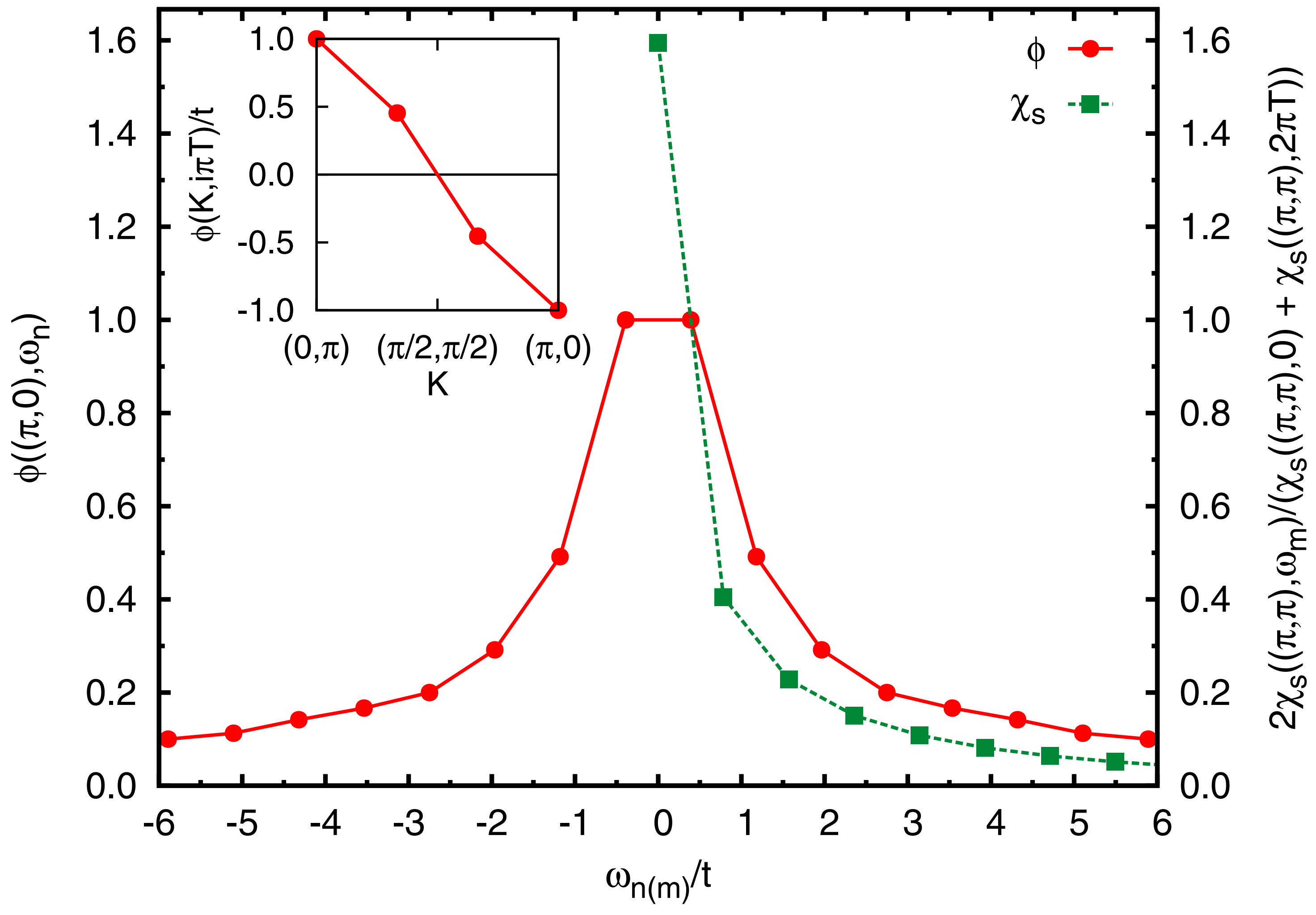
Structure of the pairing interaction



Momentum dependence



Frequency dependence



TAM et al., PRL '06, PRB '06

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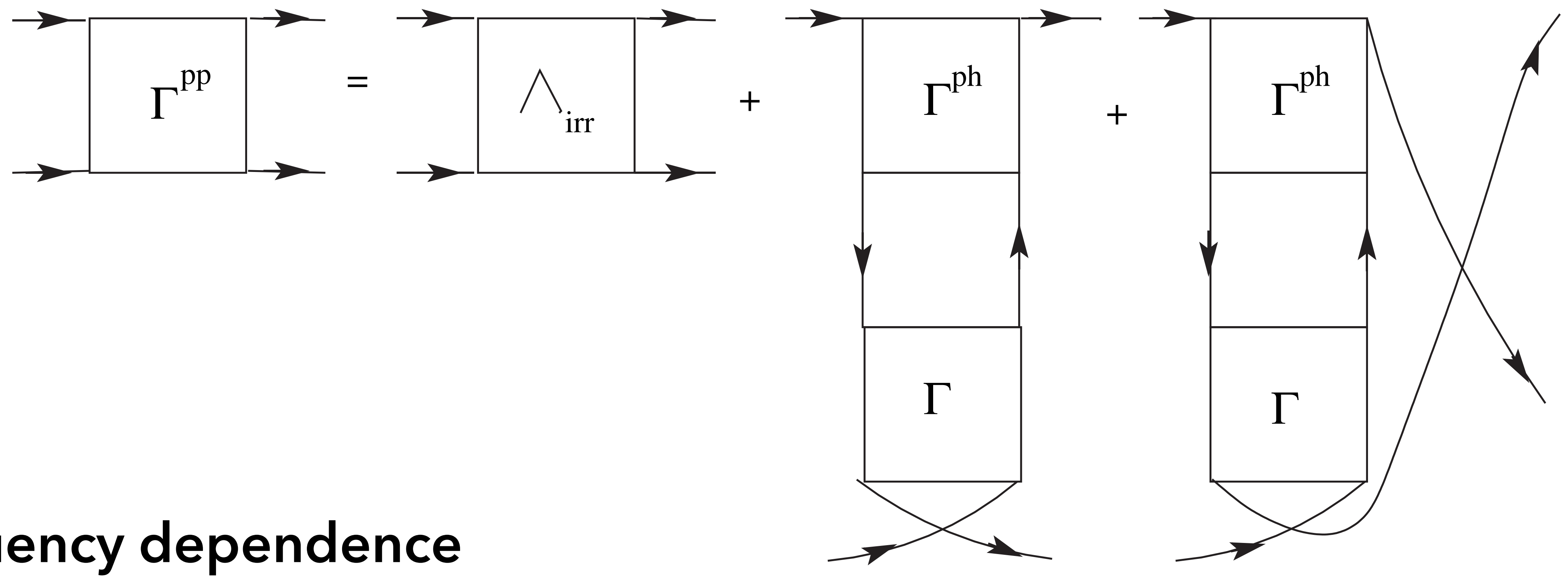

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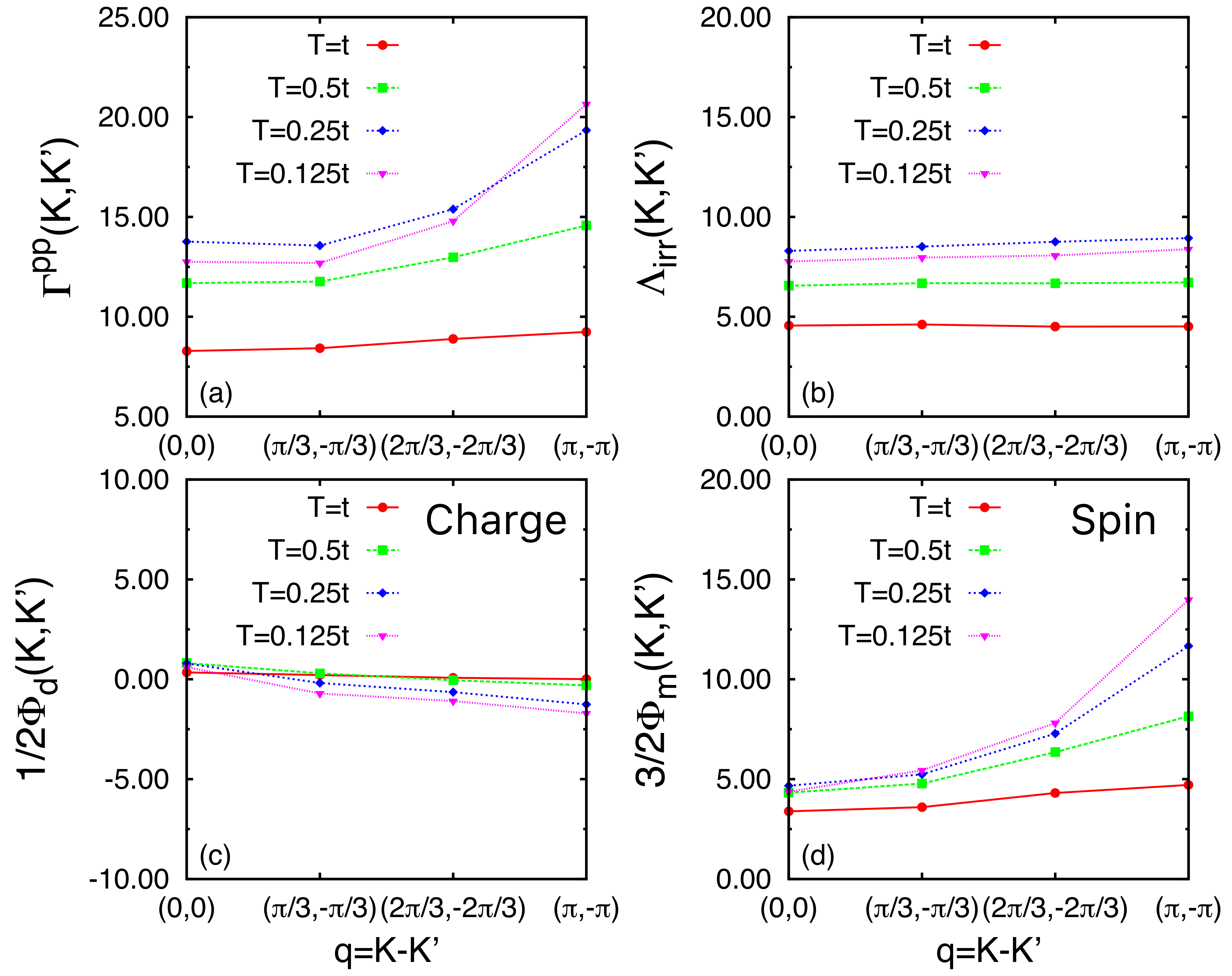

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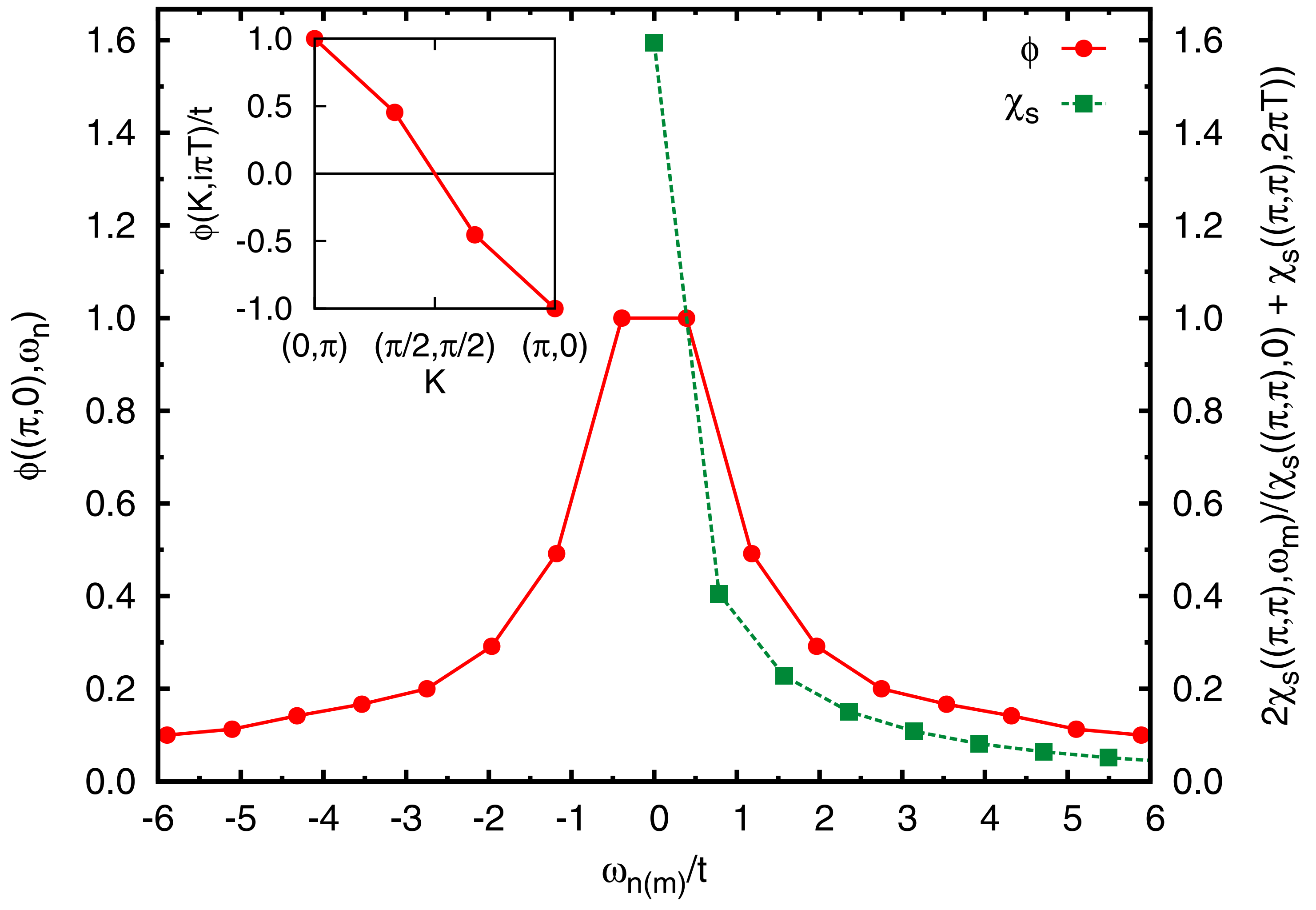

TAM et al., PRL '06, PRB '06

- Pairing interaction carries spin S=1, increases with momentum transfer, and its dynamics reflects the spin fluctuation spectrum

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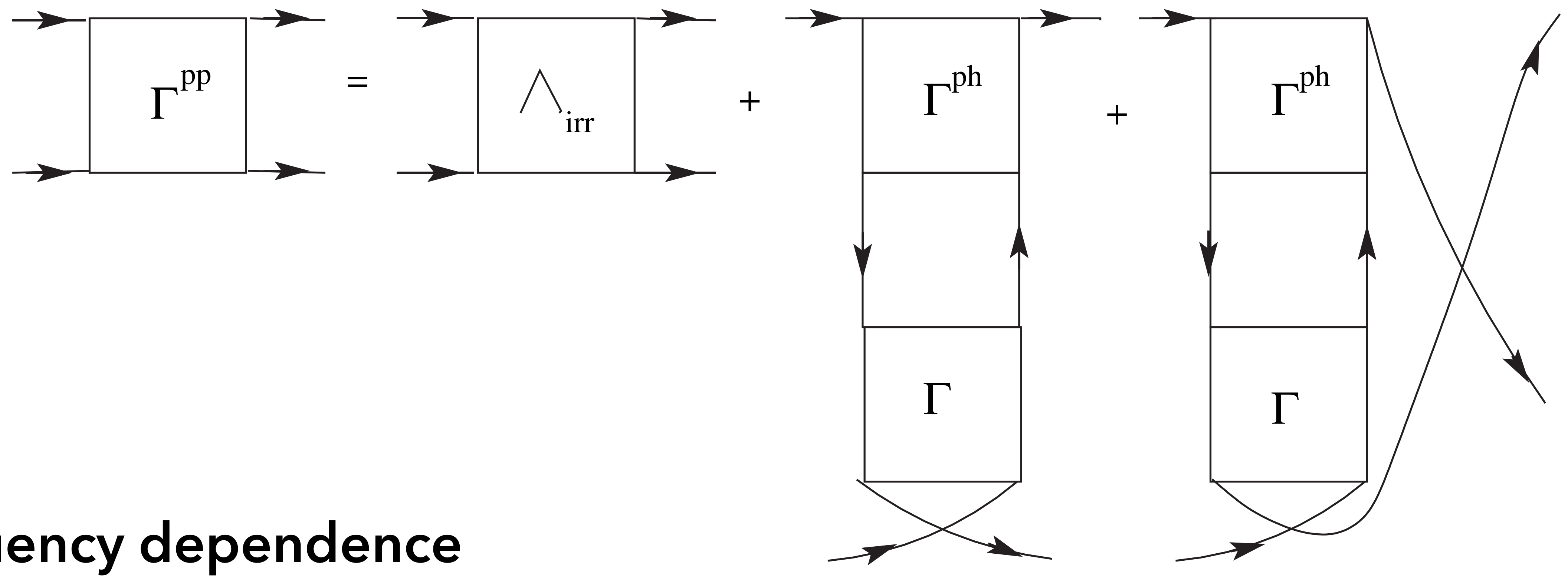

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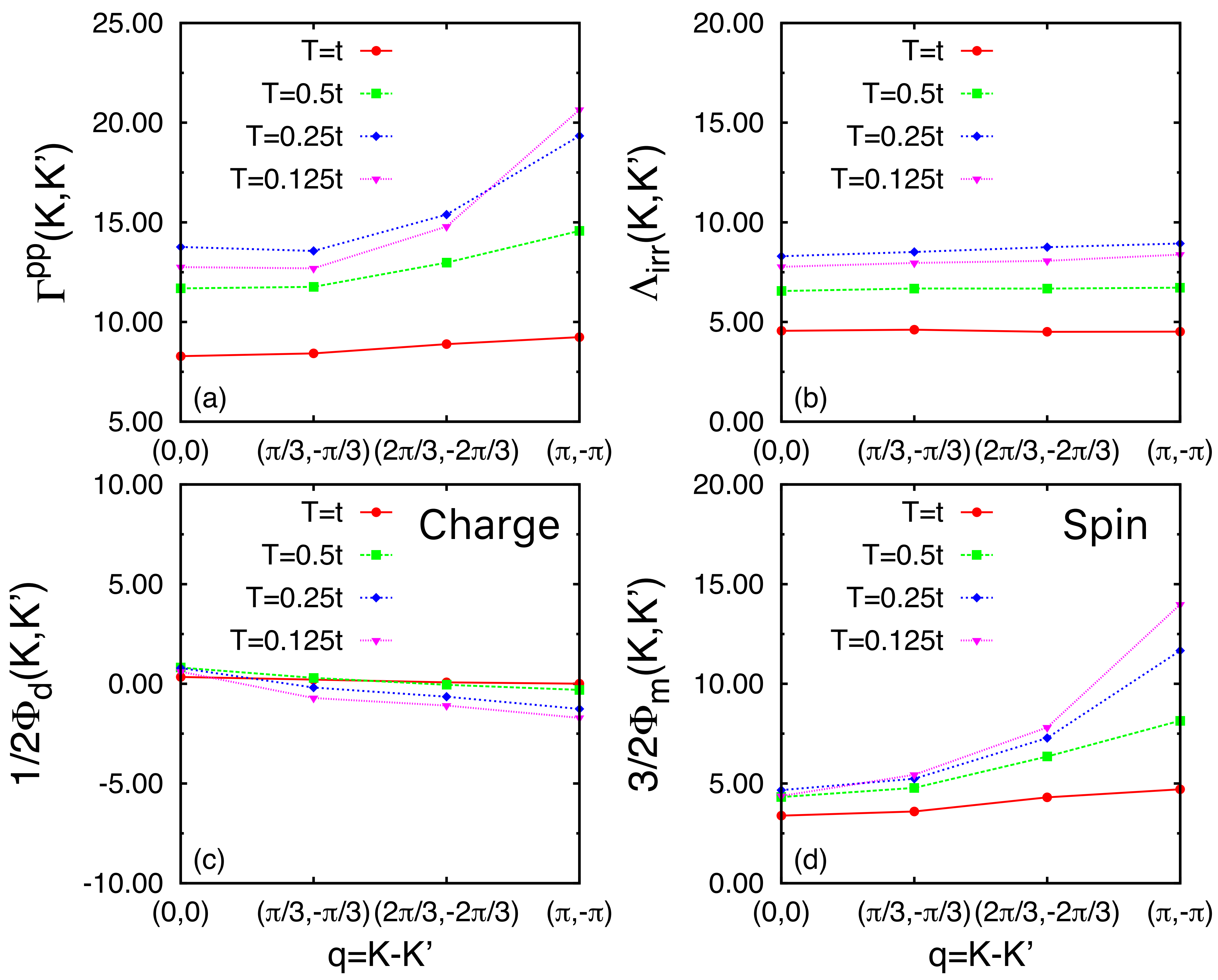

TAM et al., PRL '06, PRB '06

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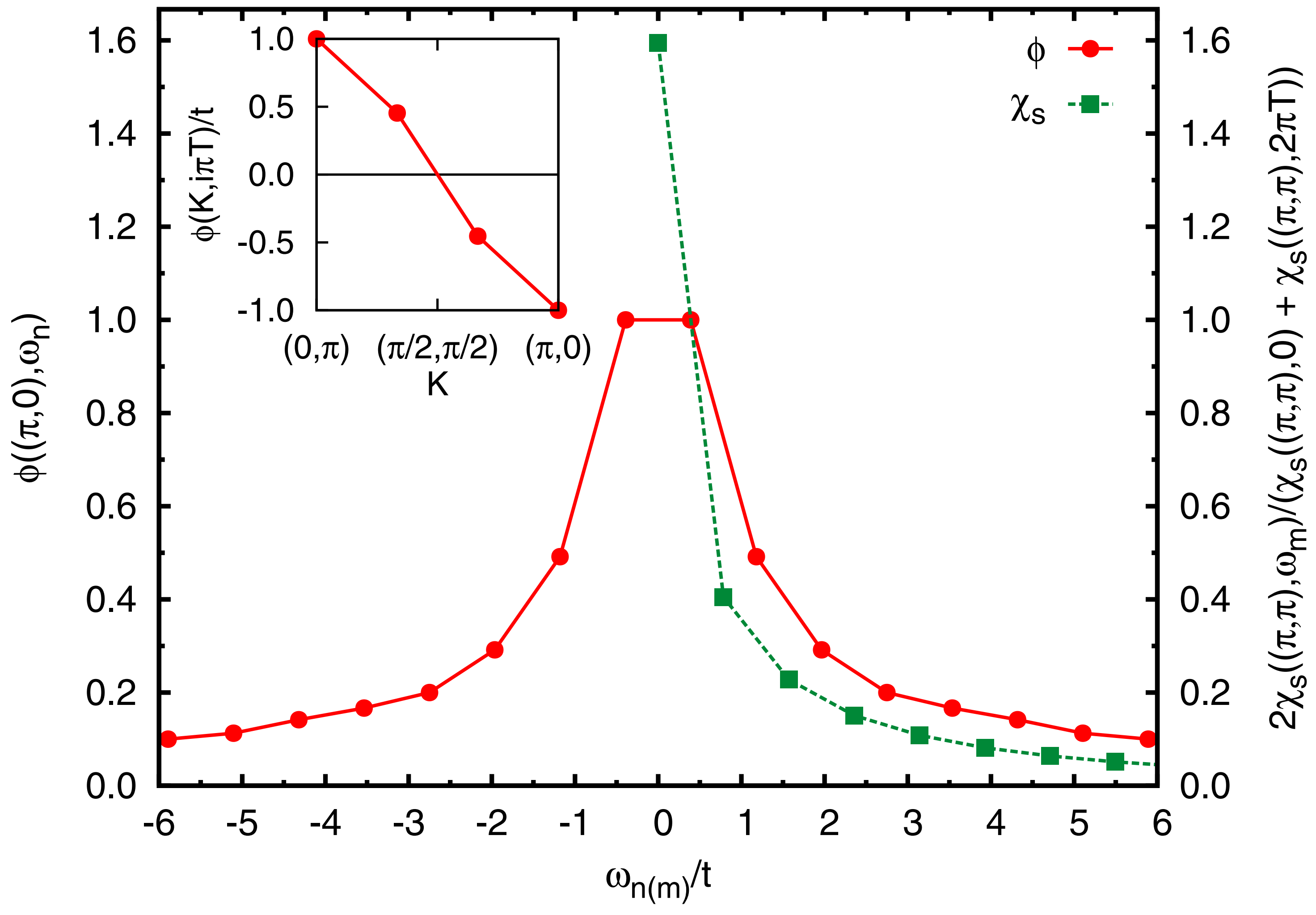
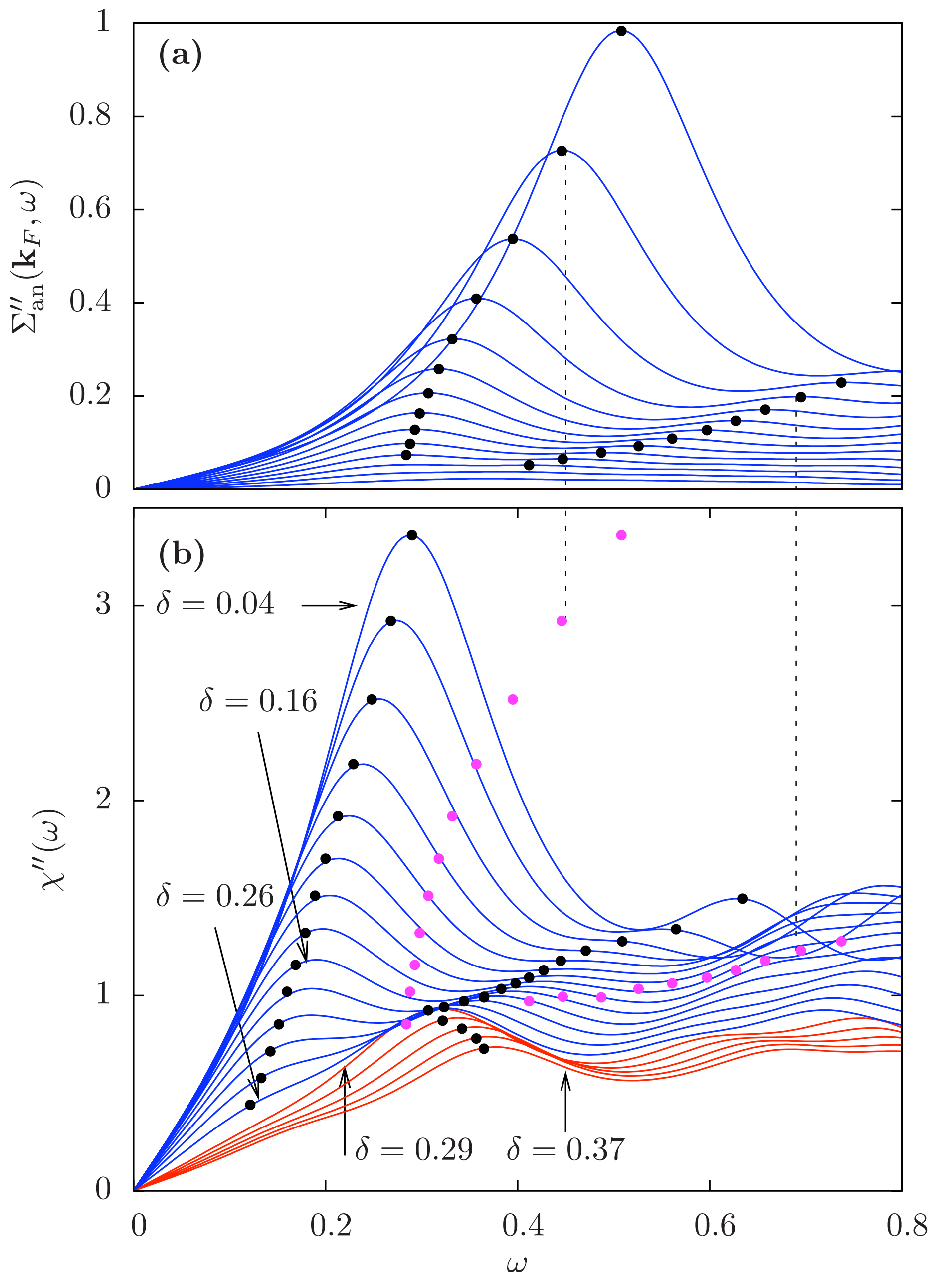


PHYSICAL REVIEW B **80**, 205109 (2009)

Pairing dynamics in strongly correlated superconductivity

B. Kyung, D. Sénéchal, and A.-M. S. Tremblay



- Pairing interaction carries spin S=1, increases with momentum transfer, and its dynamics reflects the spin fluctuation spectrum

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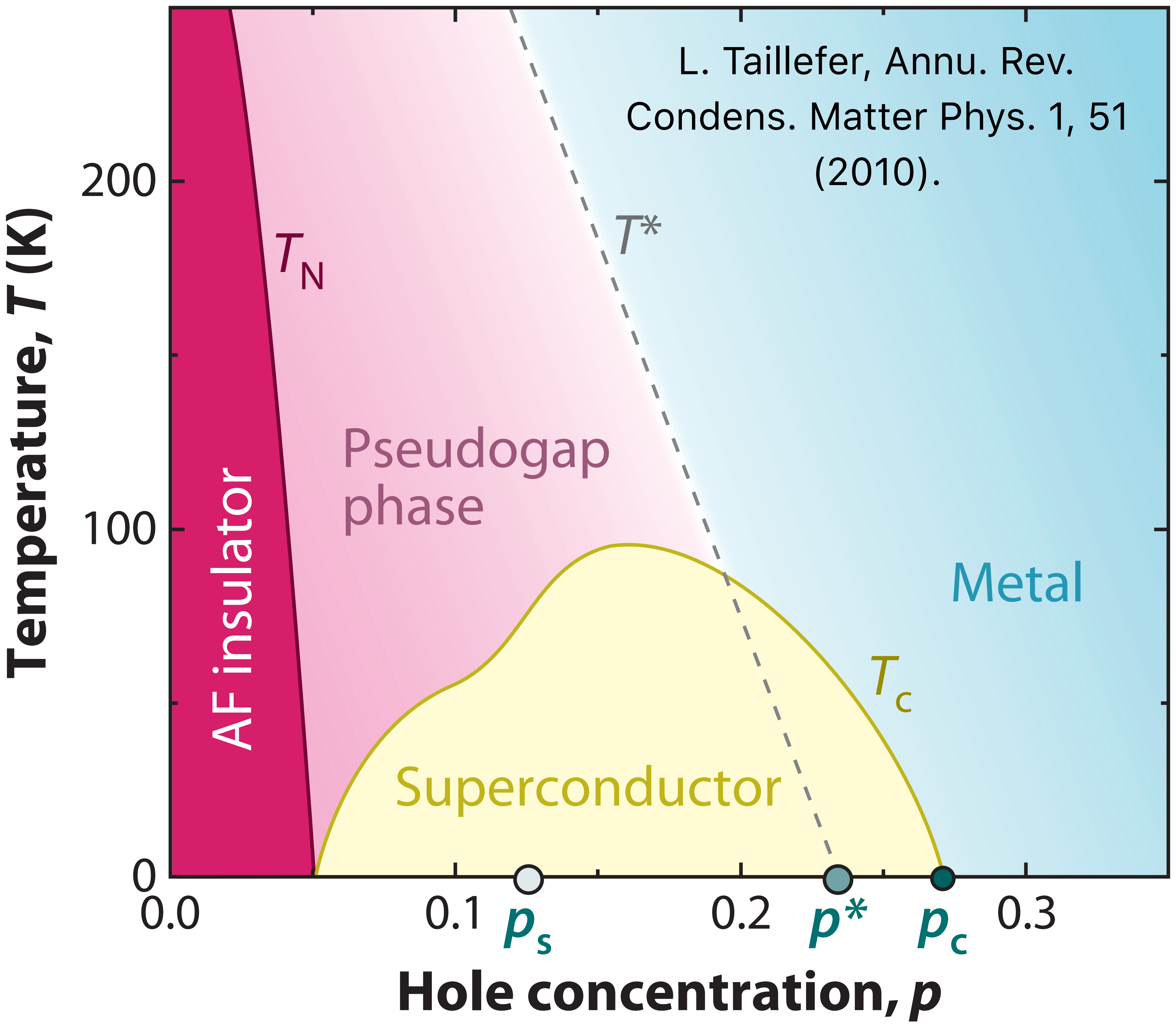
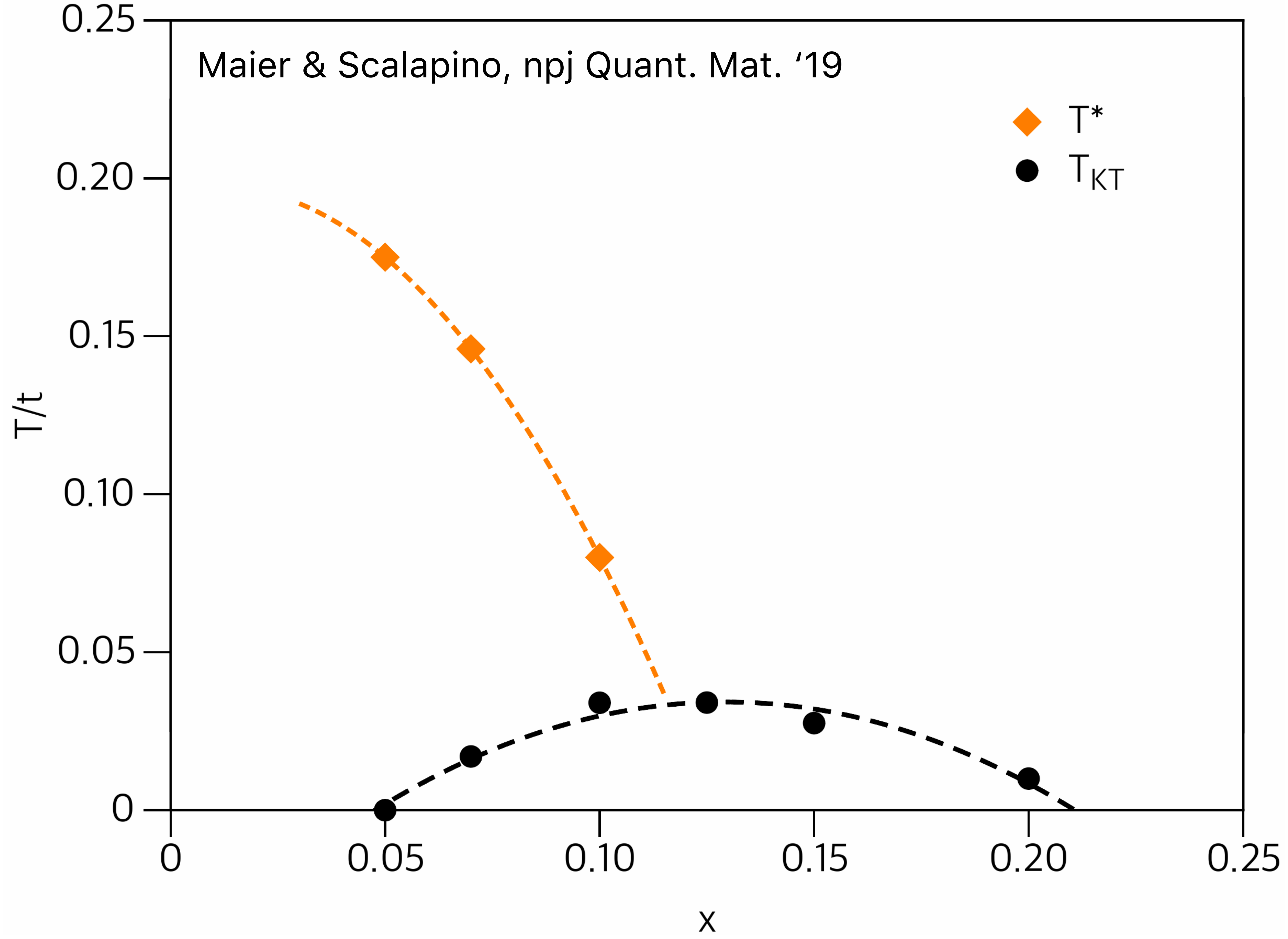
DCA phase diagram



Schematic DCA phase diagram
(12-site cluster, U=7t, t′/t=-0.15)



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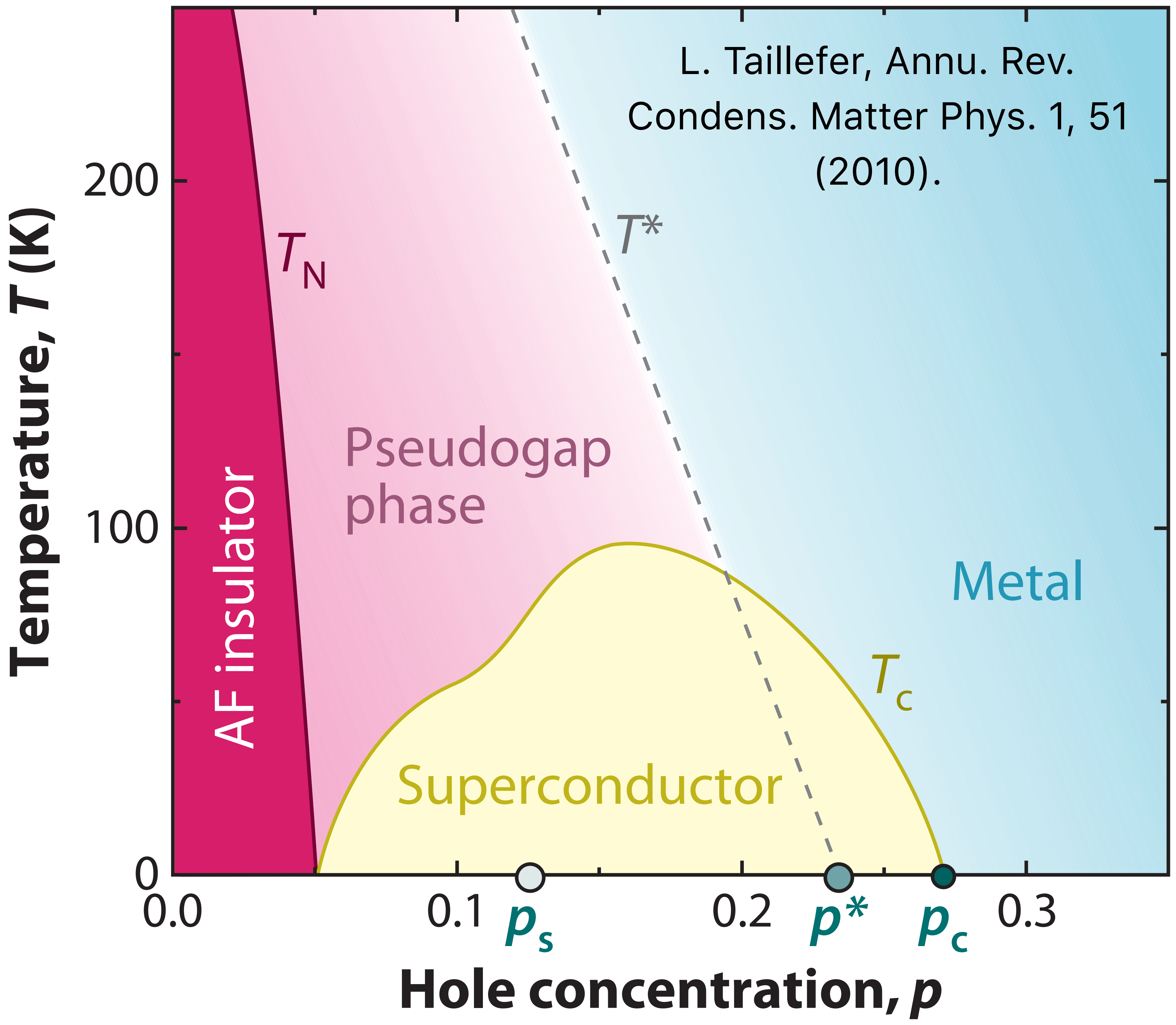

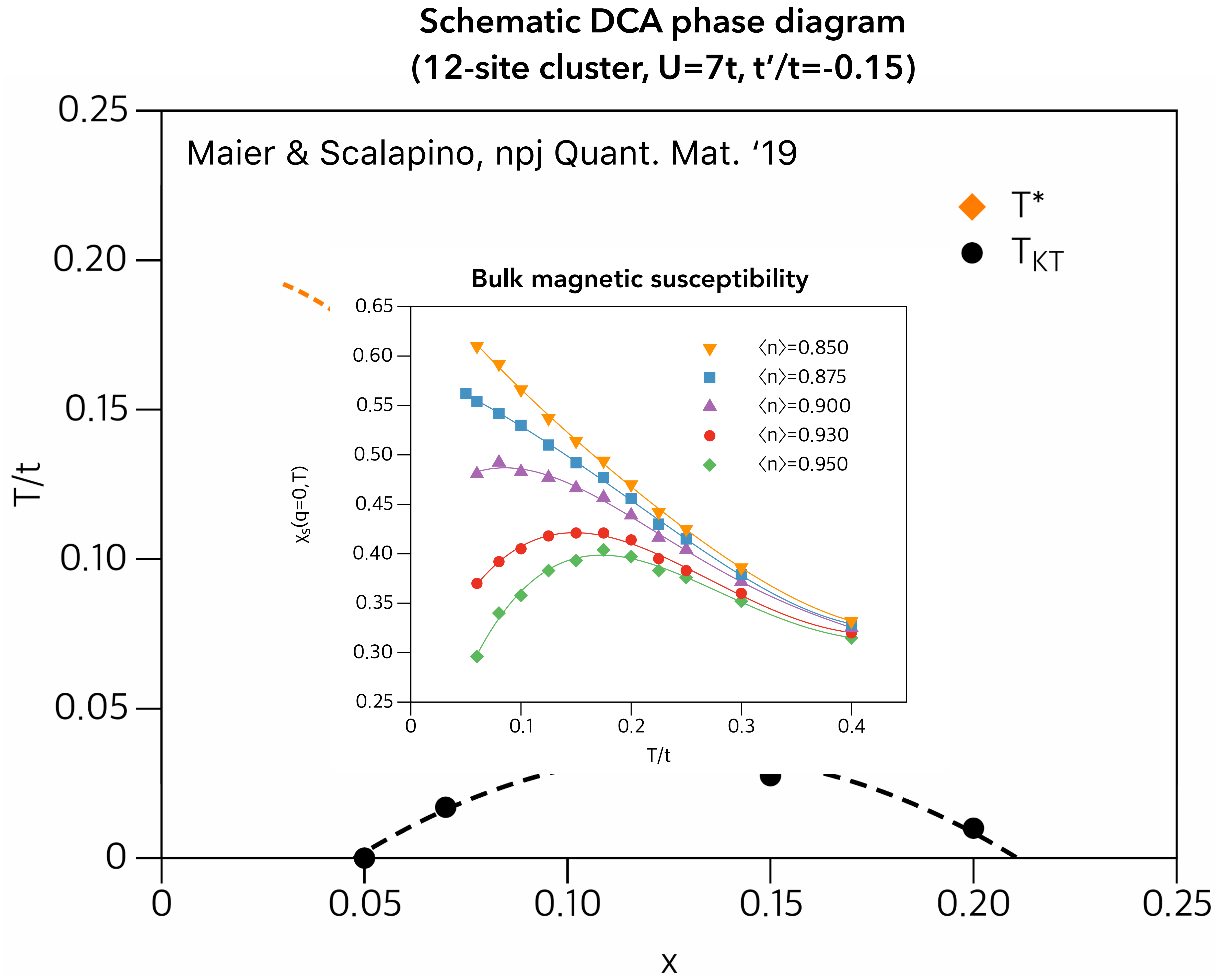

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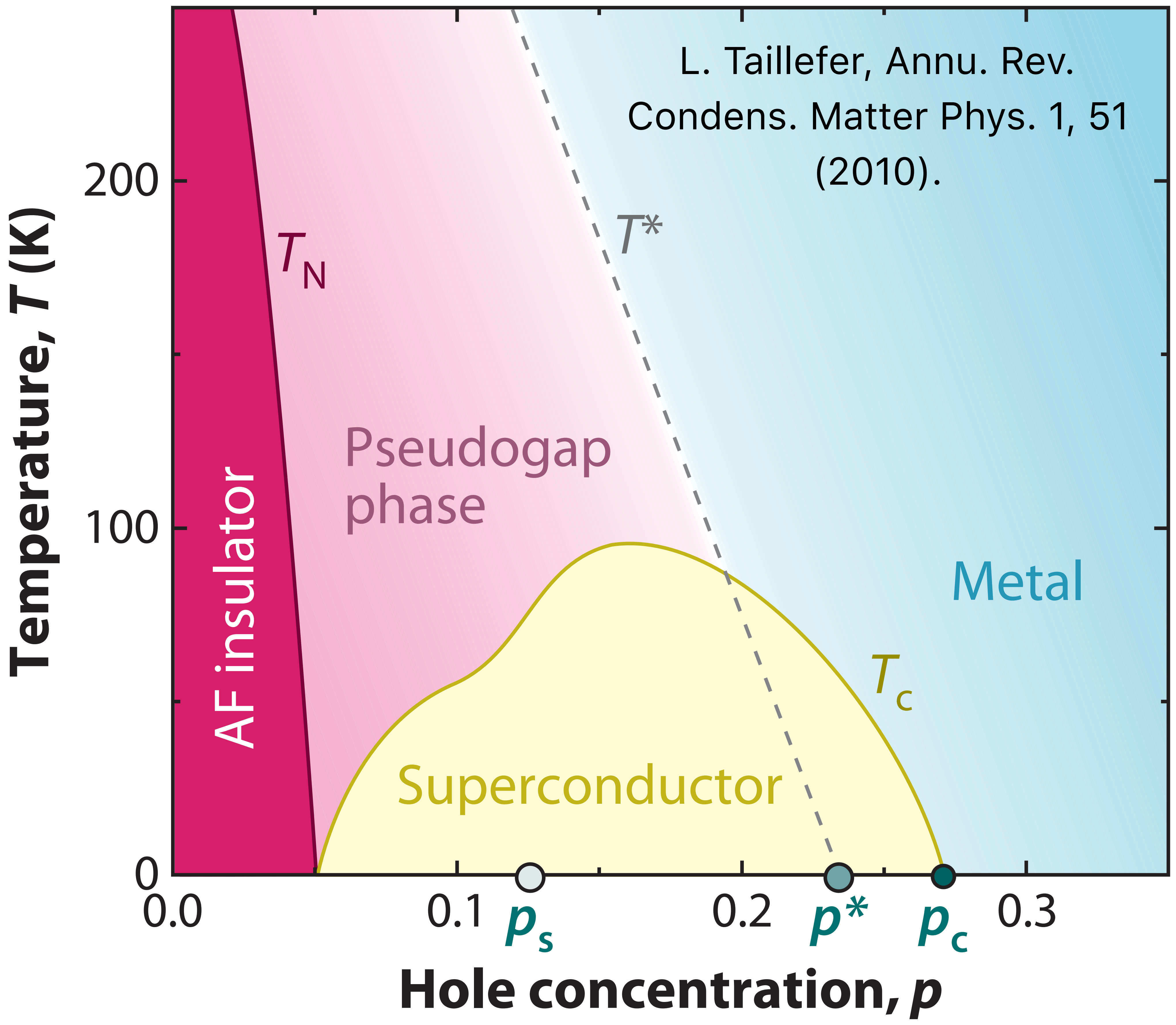
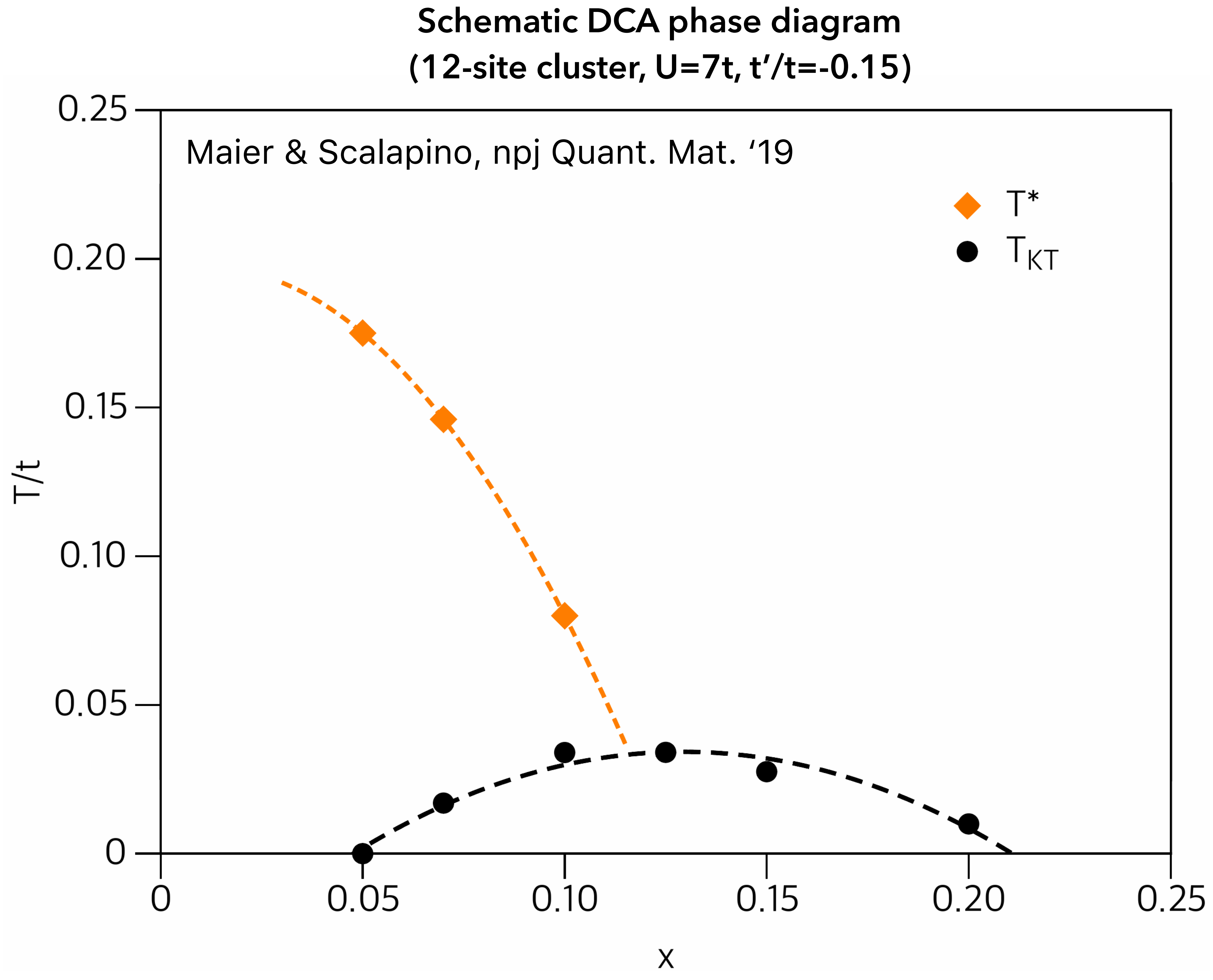
DCA phase diagram





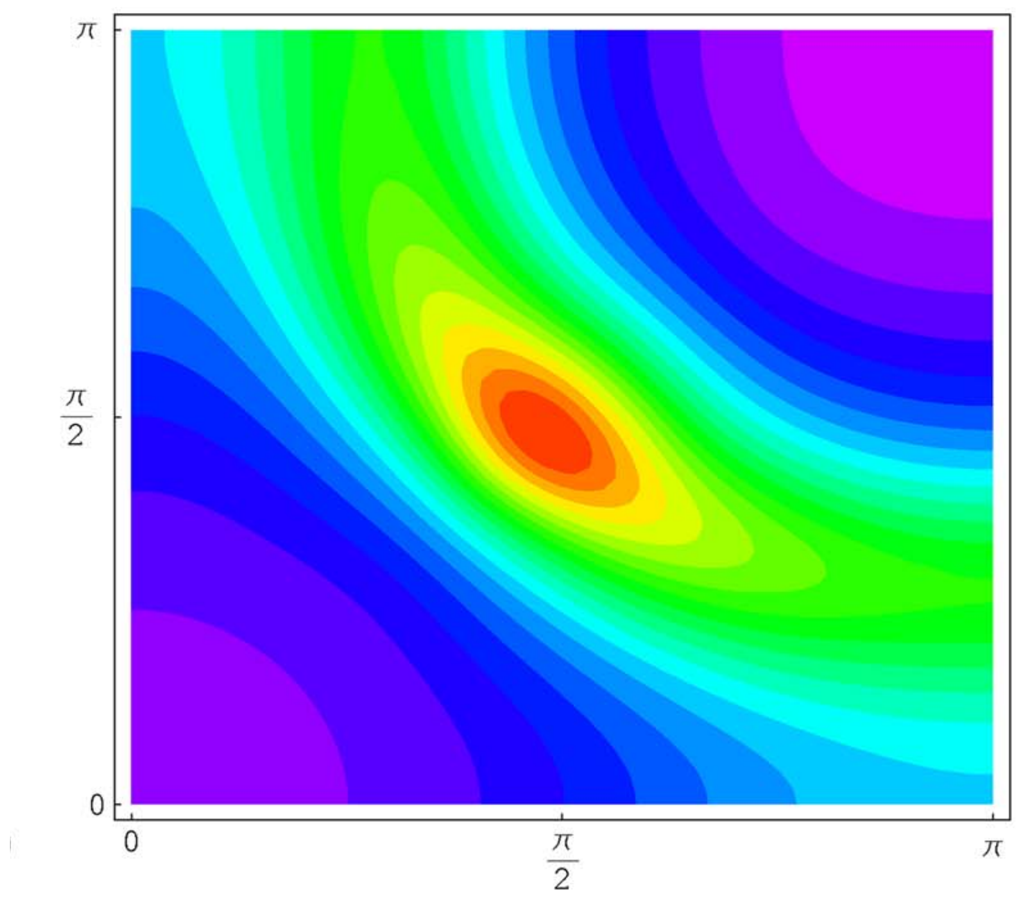
Pseudogap in the 2D Hubbard Model

PHYSICAL REVIEW B **73**, 165114 (2006)

Pseudogap induced by short-range spin correlations in a doped Mott insulator

B. Kyung, S. S. Kancharla, D. Sénéchal, and A.-M. S. Tremblay
Département de physique and Regroupement québécois sur les matériaux de pointe, Université de Sherbrooke, Sherbrooke, Québec, Canada J1K 2R1

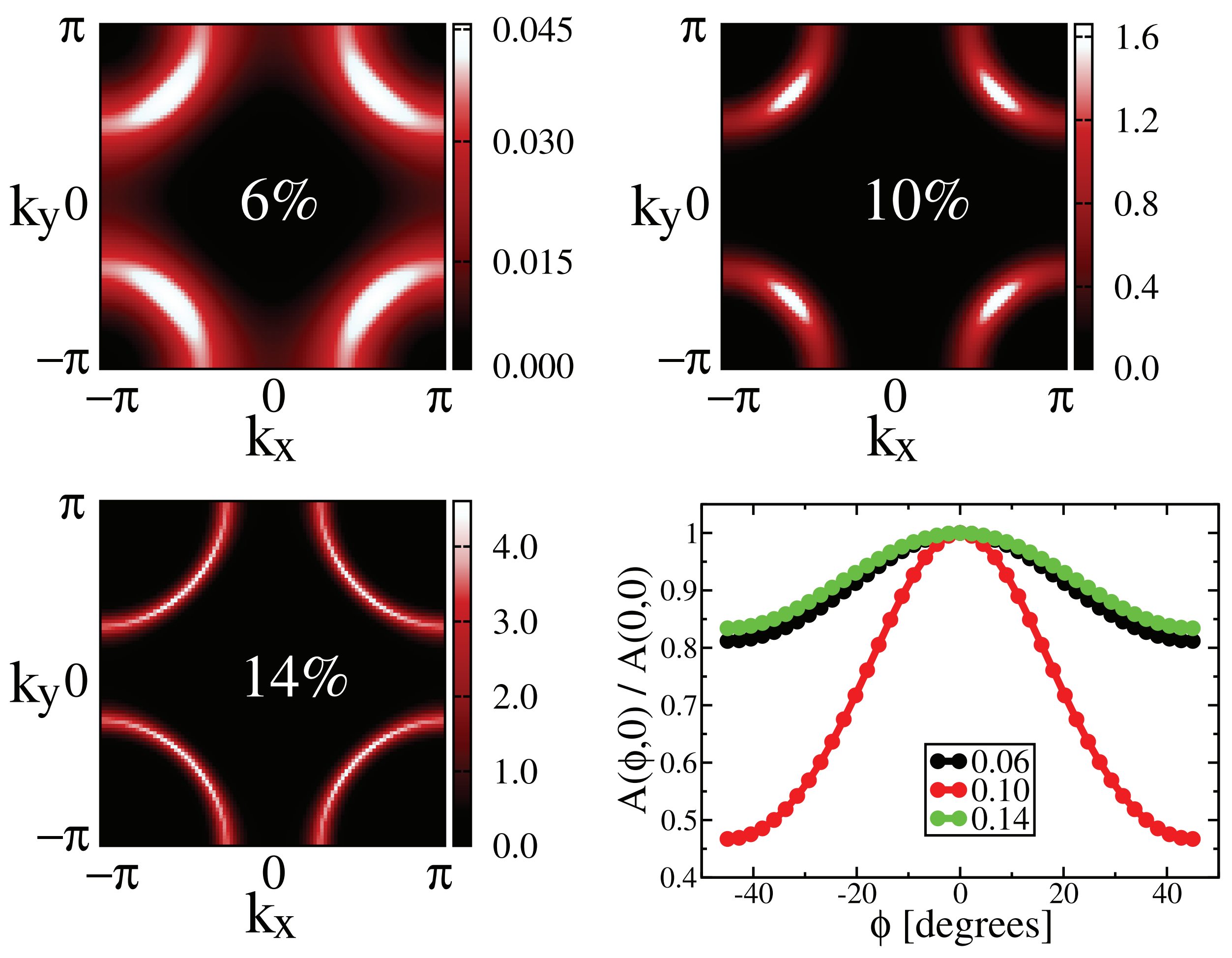
M. Civelli and G. Kotliar
Physics Department and Center for Materials Theory, Rutgers University, Piscataway, New Jersey 08855, USA
(Received 27 January 2006; revised manuscript received 21 February 2006; published 13 April 2006)



epl A LETTERS JOURNAL EXPLORING THE FRONTIERS OF PHYSICS
March 2009
EPL, **85** (2009) 57009
www.epljournal.org
doi: 10.1209/0295-5075/85/57009

Valence bond dynamical mean-field theory of doped Mott insulators with nodal/antinodal differentiation

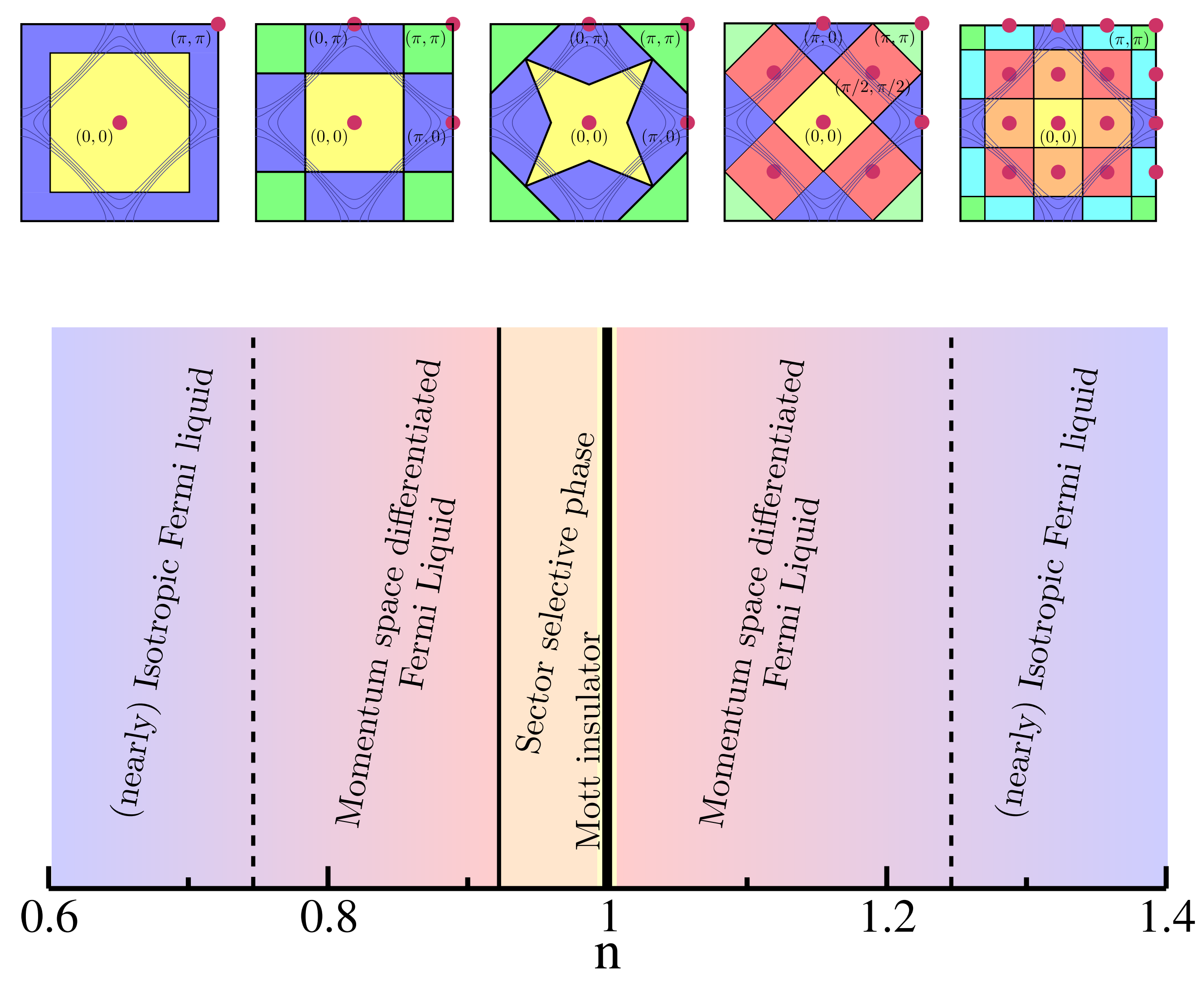
M. FERRERO[1], P. S. CORNAGLIA[1,2], L. DE LEO[1], O. PARCOLLET[3], G. KOTLIAR[4] and A. GEORGES[1]



PHYSICAL REVIEW B **82**, 155101 (2010)

Momentum-space anisotropy and pseudogaps: A comparative cluster dynamical mean-field analysis of the doping-driven metal-insulator transition in the two-dimensional Hubbard model

E. Gull,[1] M. Ferrero,[2] O. Parcollet,[3] A. Georges,[2,4] and A. J. Millis[1]



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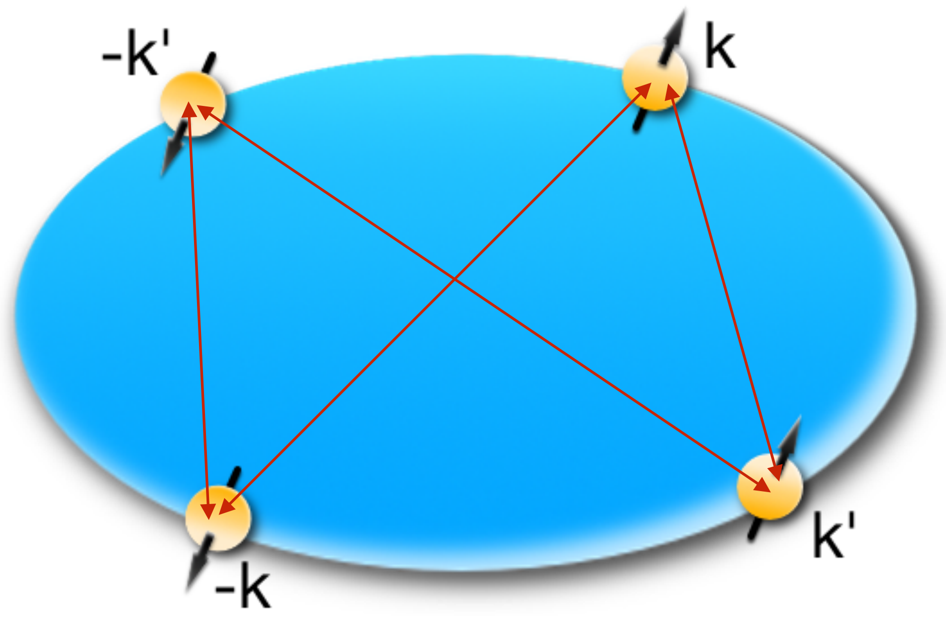
Pairing in a dry Fermi sea

Normal metal: Cooper log instability



$$P(T) \sim \frac{1}{1 - \lambda(T)}$$

$$\lambda(T) = VP_0(T)$$

$$P_0(T) \sim \log(a/T)$$

- Pairing interaction V is set at high T and SC instability arises from Cooper log divergence of pair propagator $P_0(T)$

Pairing in a dry Fermi sea

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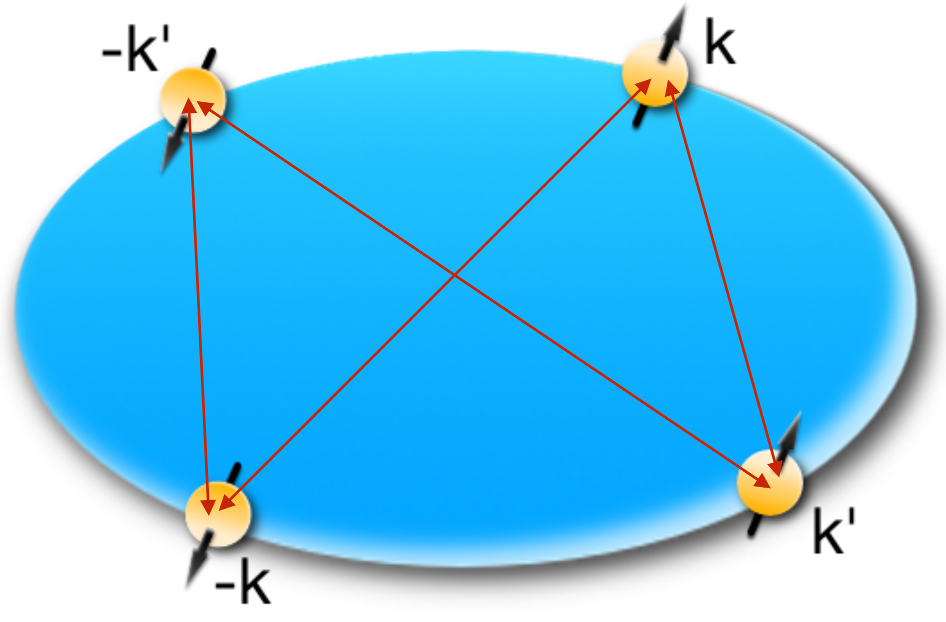

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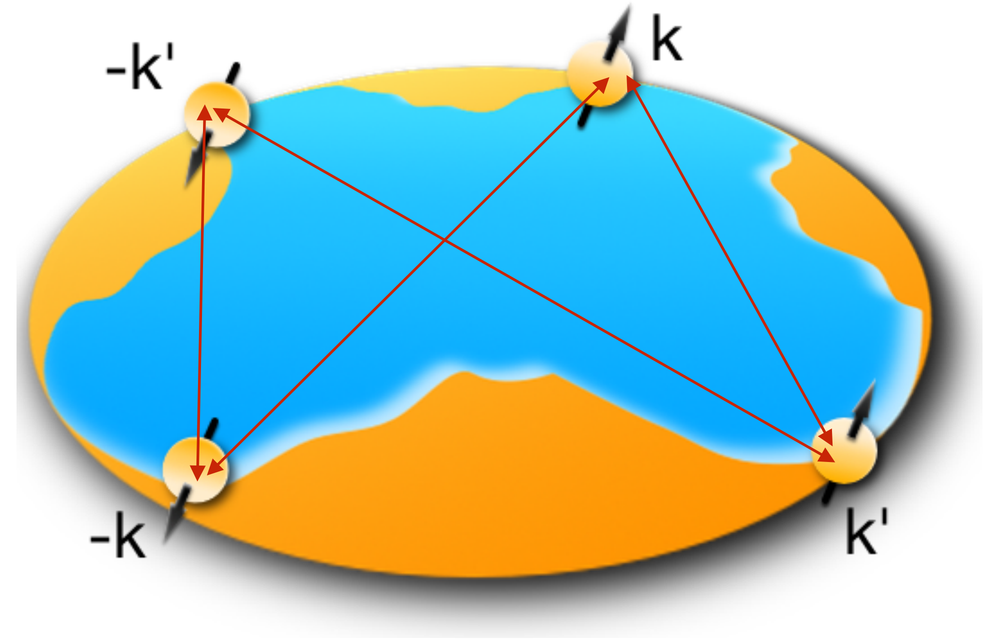
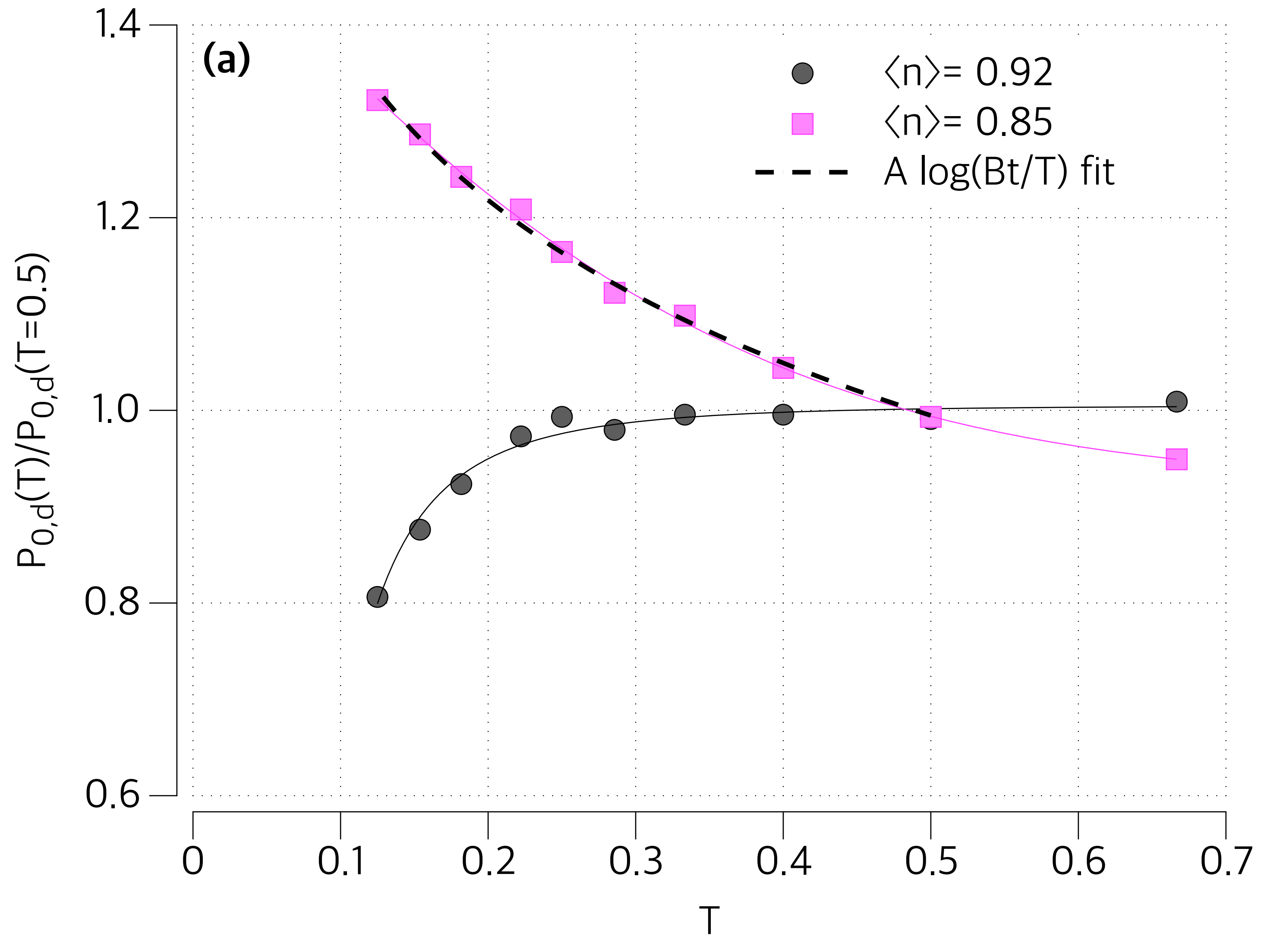
- **Pairing interaction V is set at high T and SC instability arises from Cooper log divergence of pair propagator P_0(T)**

Cuprate pseudogap phase: Absence of Cooper log divergence





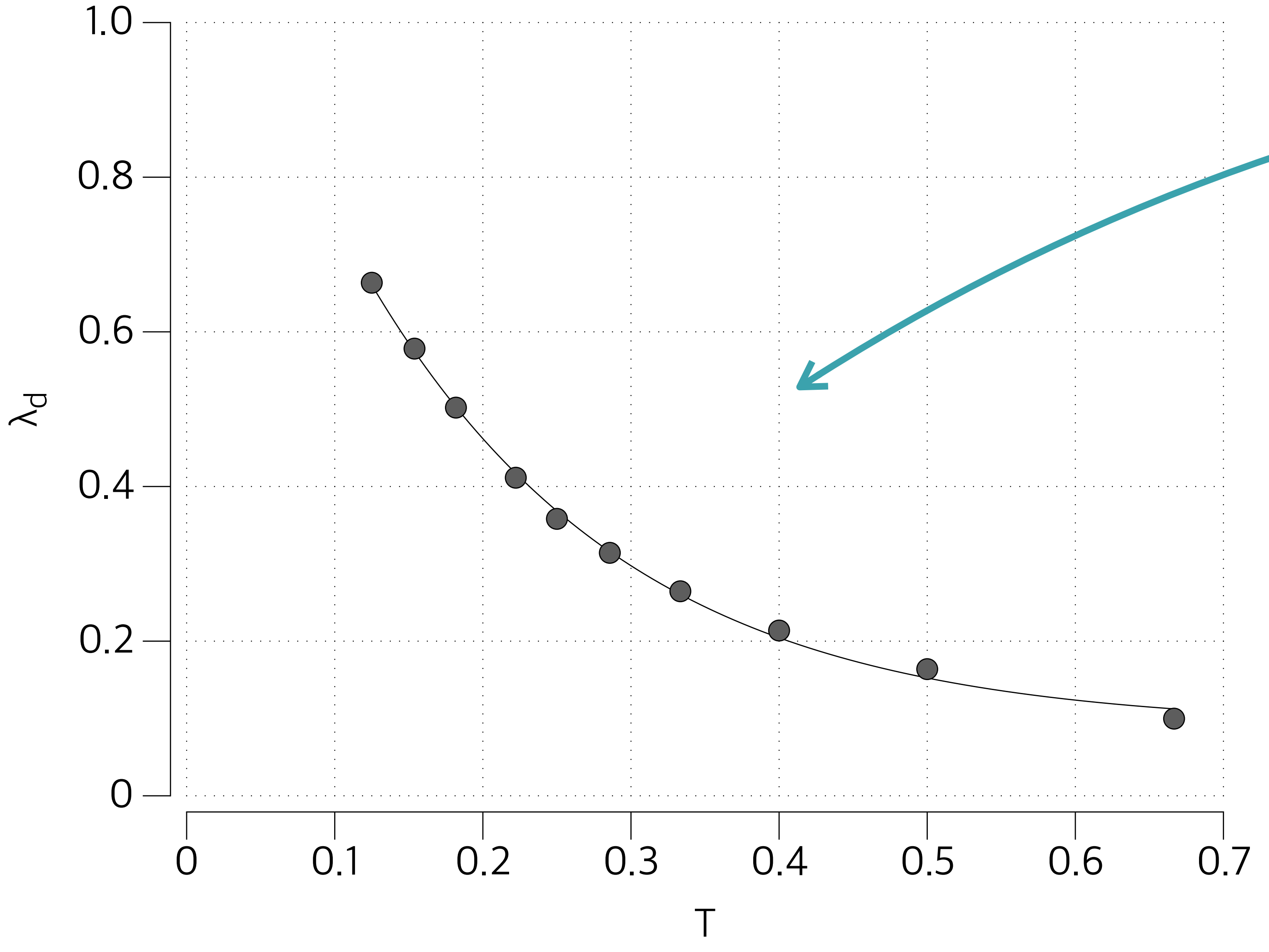
- **Cooper log instability is absent and $P_{d,0}$(T) decreases for T < T***

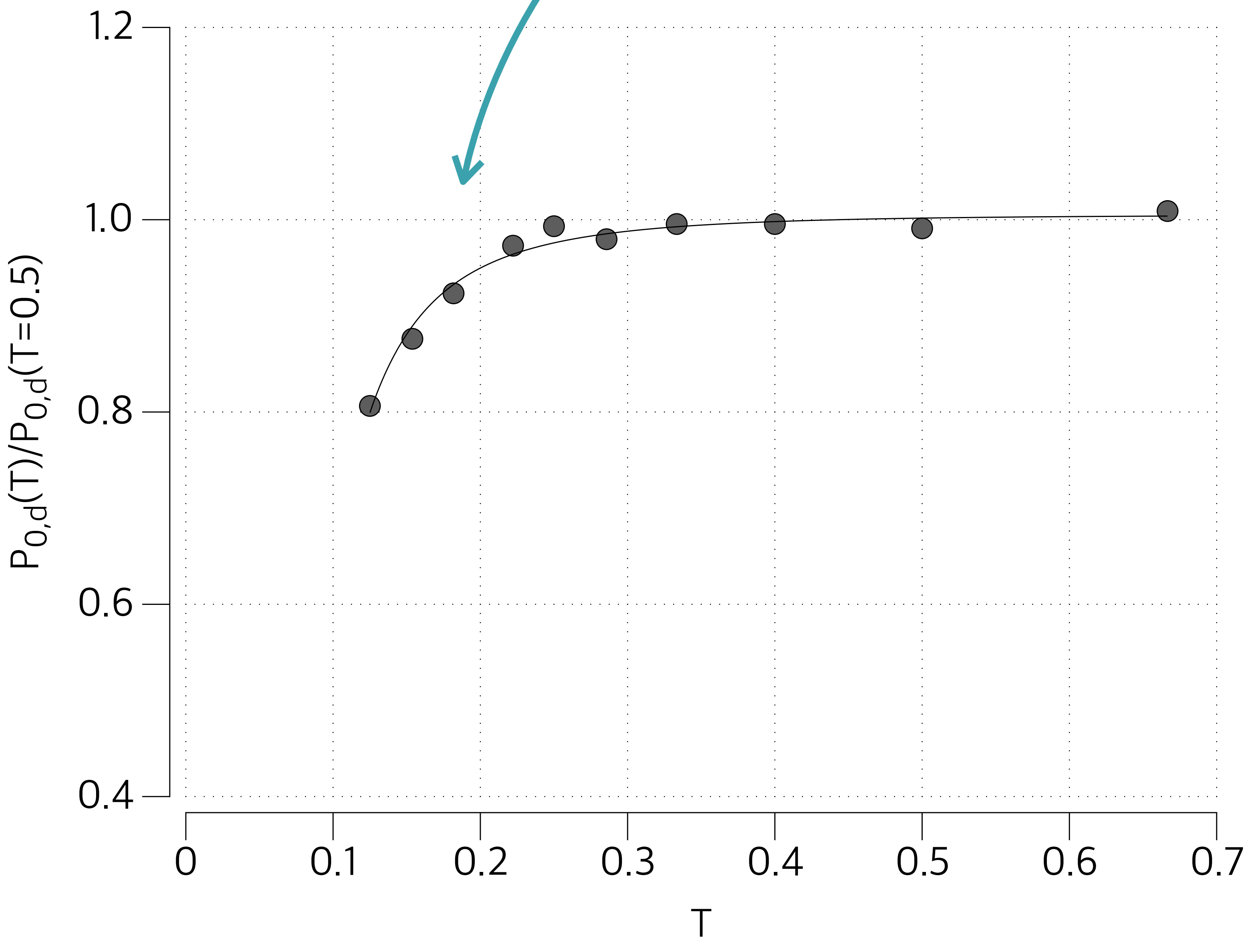
TAM *et al.*, Nat. Comm. '16

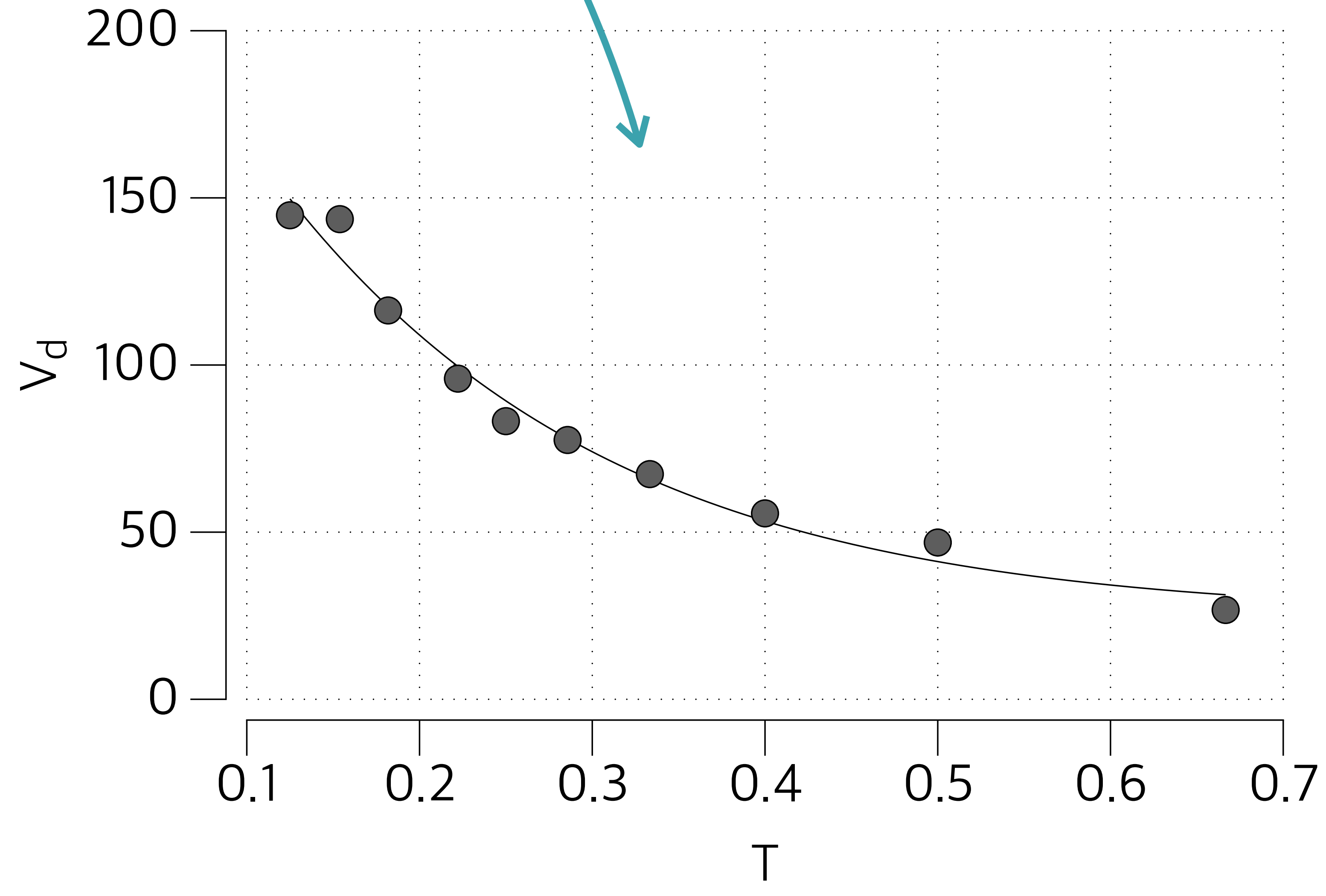
Pairing interaction in pseudogap regime

$$\lambda_d(T) \approx P_{0,d}(T)V_d(T)$$

TAM *et al.*, Nat. Comm. '16



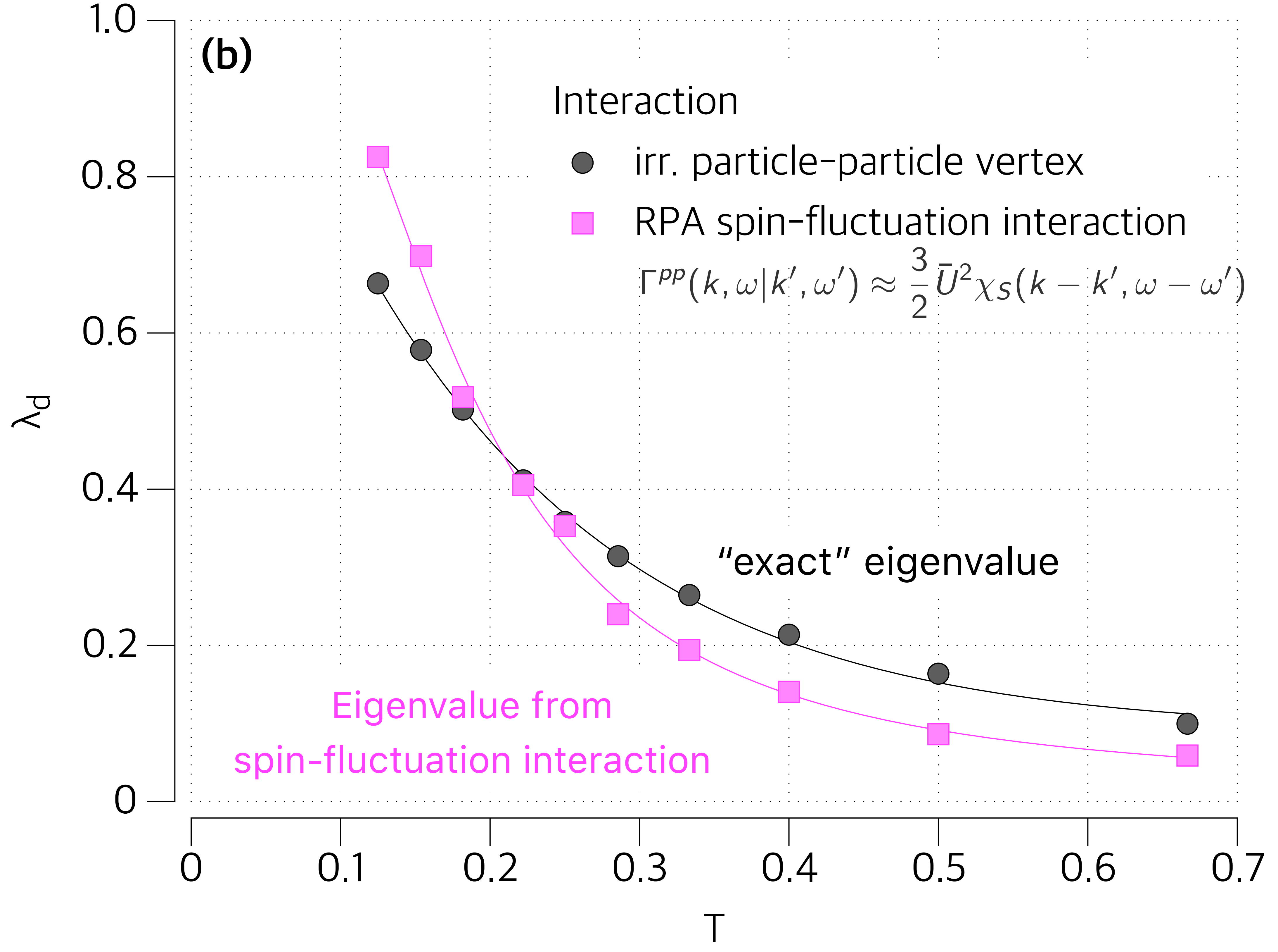




- **In the pseudogap regime, it is the pairing interaction $V_d(T)$ that increases when T decreases**

Spin-fluctuation interaction

d-wave eigenvalue (Hubbard model)



- **Spin-fluctuation strength increases similar to the d-wave pairing kernel as T is lowered**

TAM *et al.*, Nat. Comm. '16

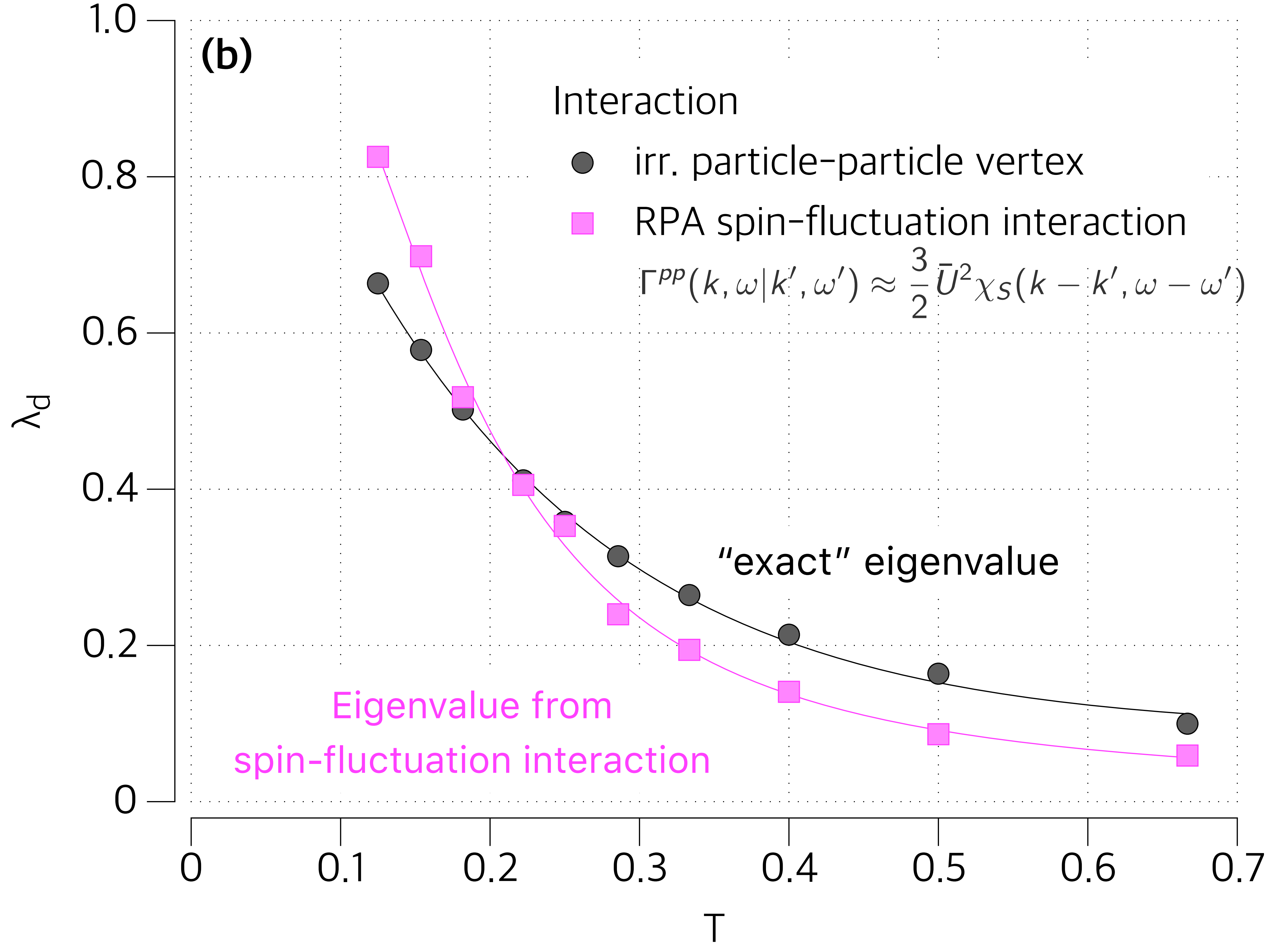
Spin-fluctuation interaction

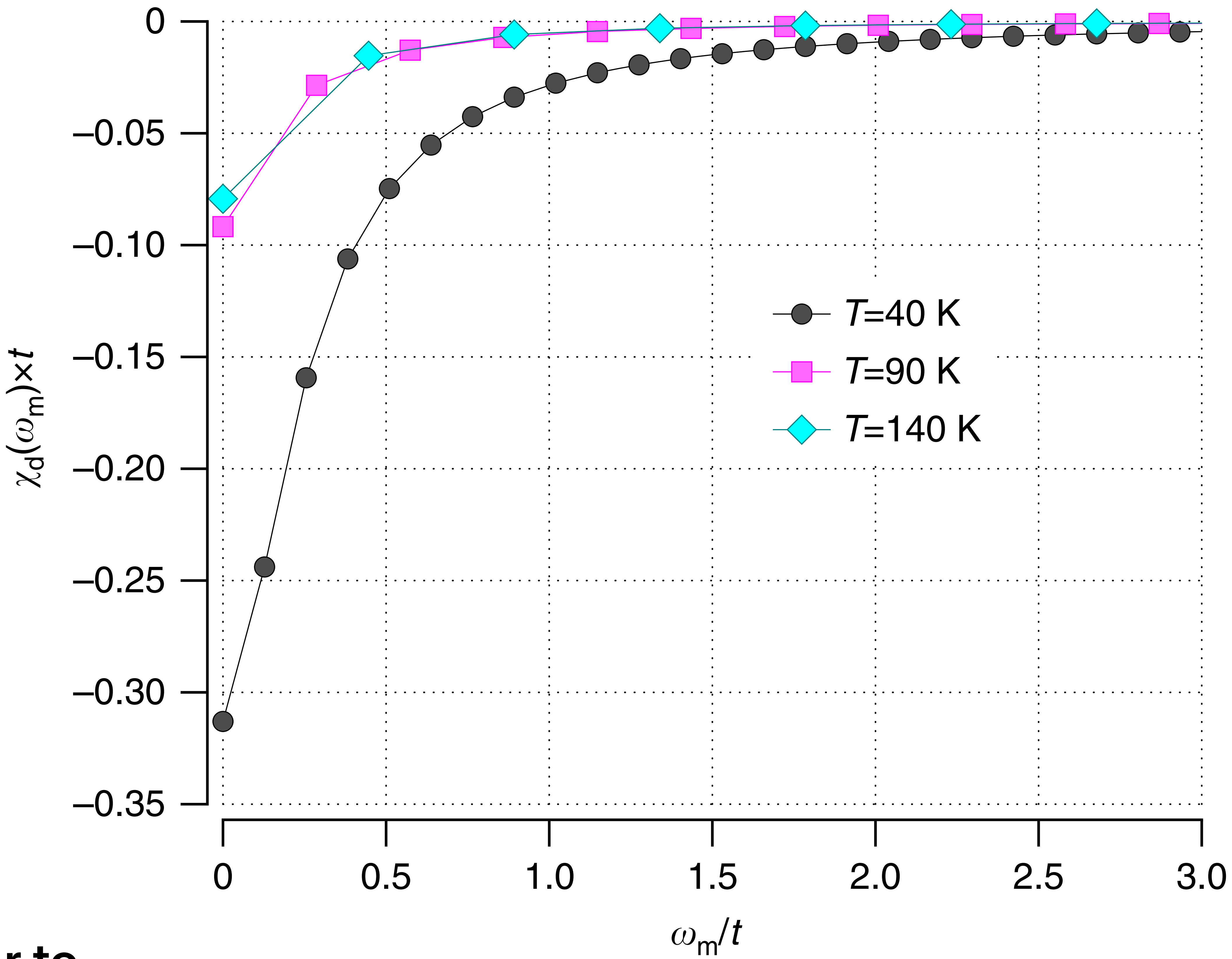
$$\chi_{\mathrm{RPA}}(q,\omega_m) = \frac{\chi_0(q,\omega_m)}{1-\bar{U}\chi_0(q,\omega_m)}$$

$$\chi_0(q,\omega_m) = -\frac{T}{N}\sum_{k,\omega_n} G(k+q,\omega_n+\omega_m)G(k,\omega_n)$$

From ARPES data on Bi2212 (T_c~90 K)

d-wave eigenvalue (Hubbard model)

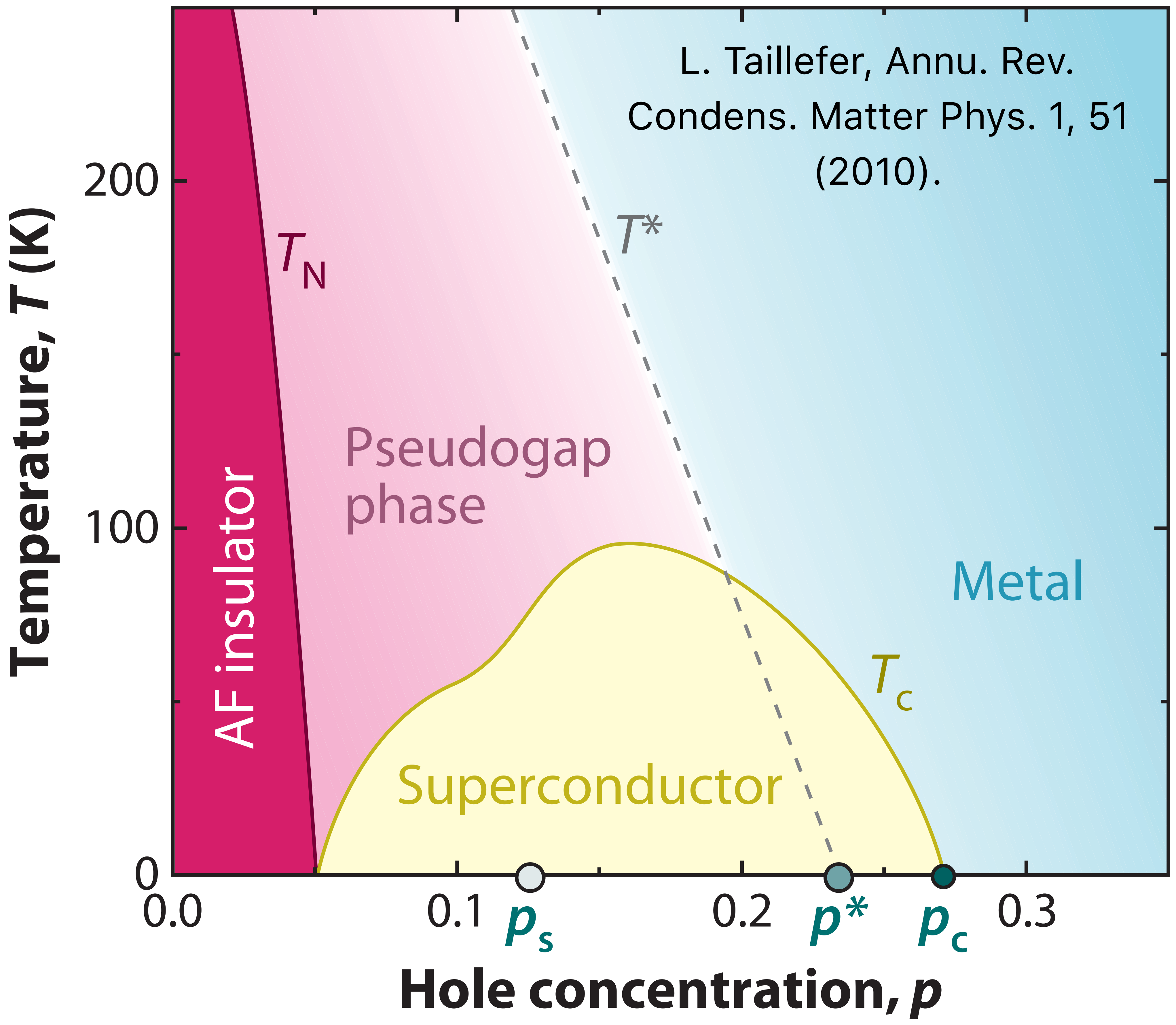




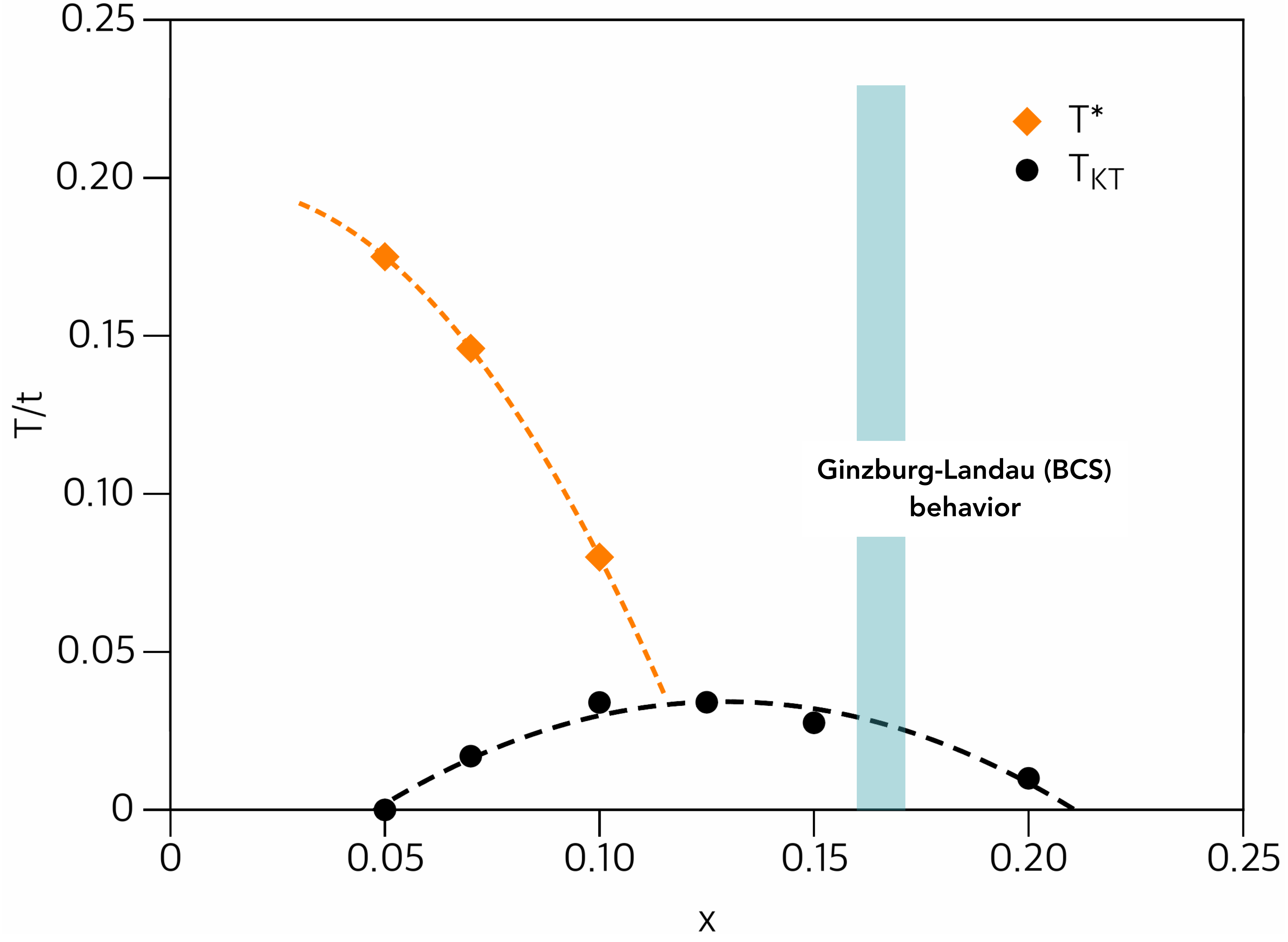
- Spin-fluctuation strength increases similar to the d-wave pairing kernel as T is lowered

TAM *et al.*, Nat. Comm. '16

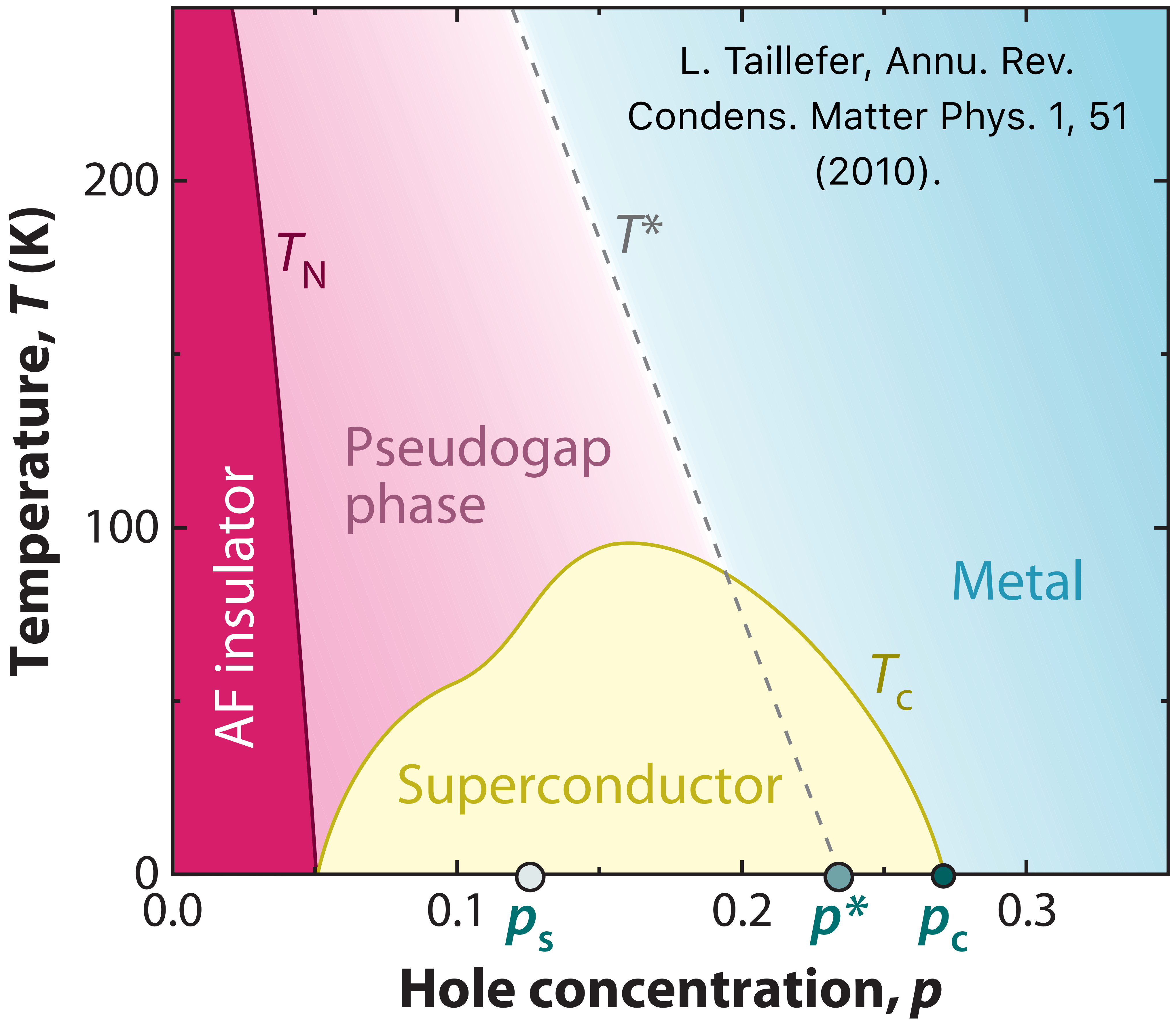
Nature of pair-field fluctuations across the superconducting dome

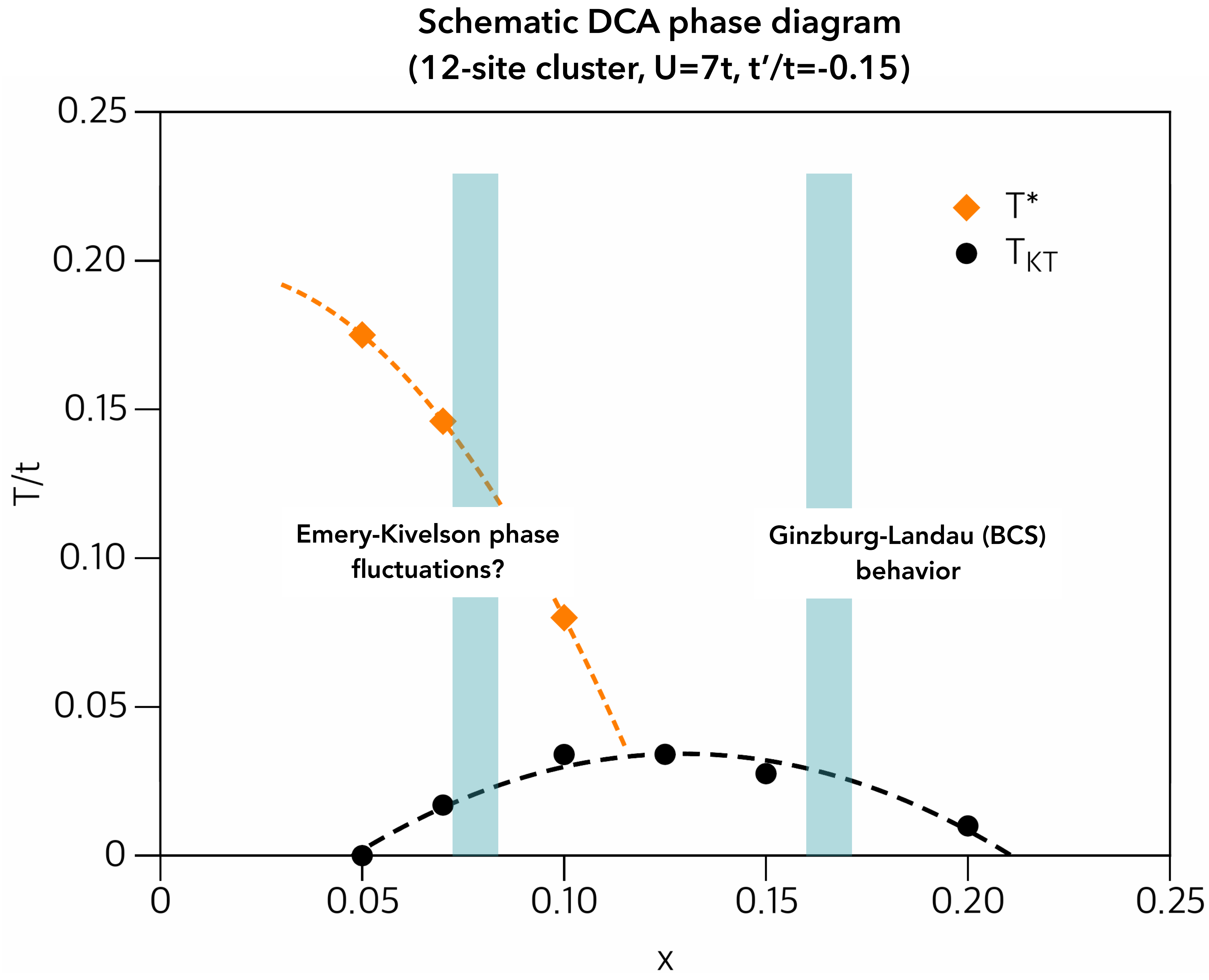


Schematic DCA phase diagram
(12-site cluster, U=7t, t'/t=-0.15)



Nature of pair-field fluctuations across the superconducting dome

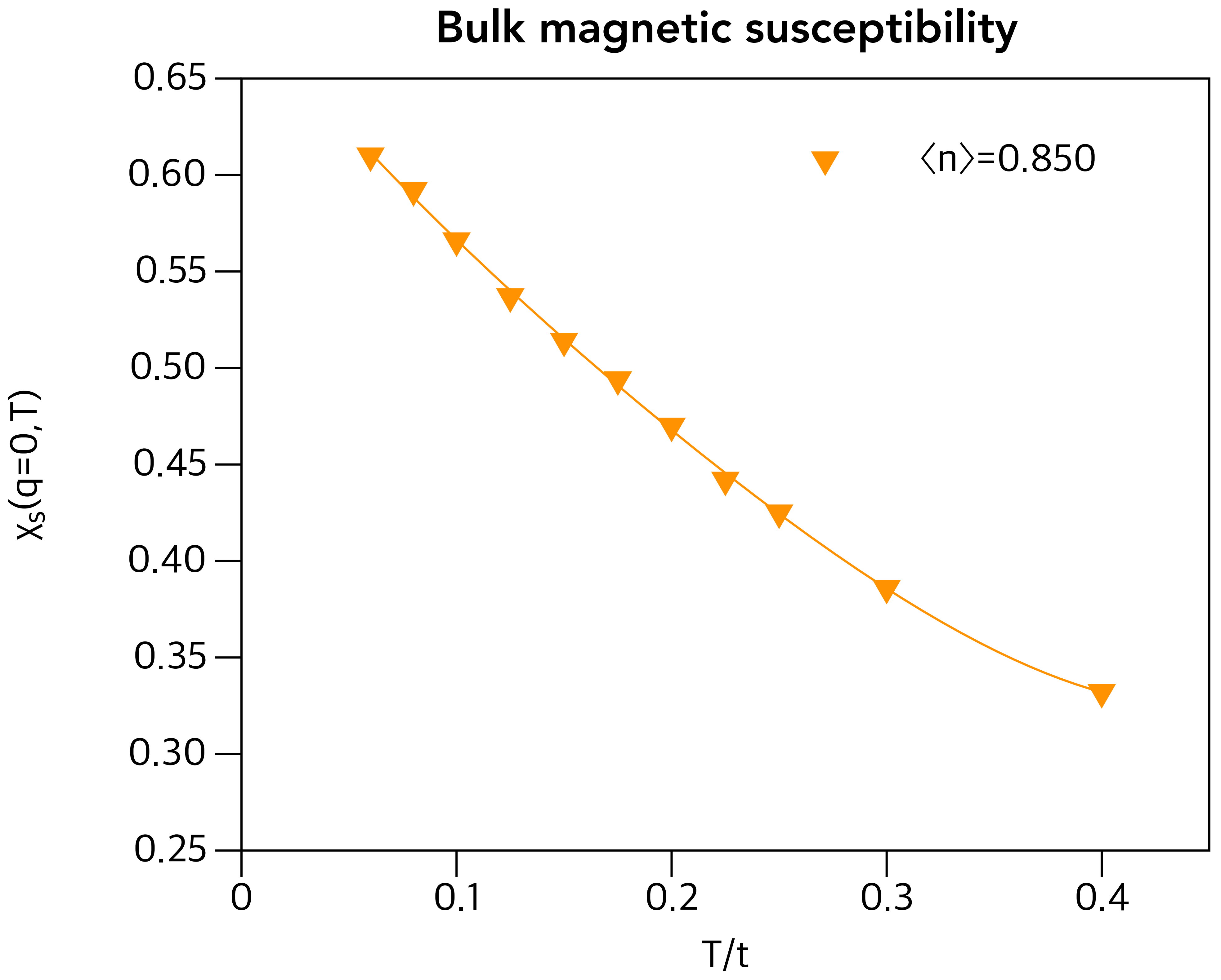


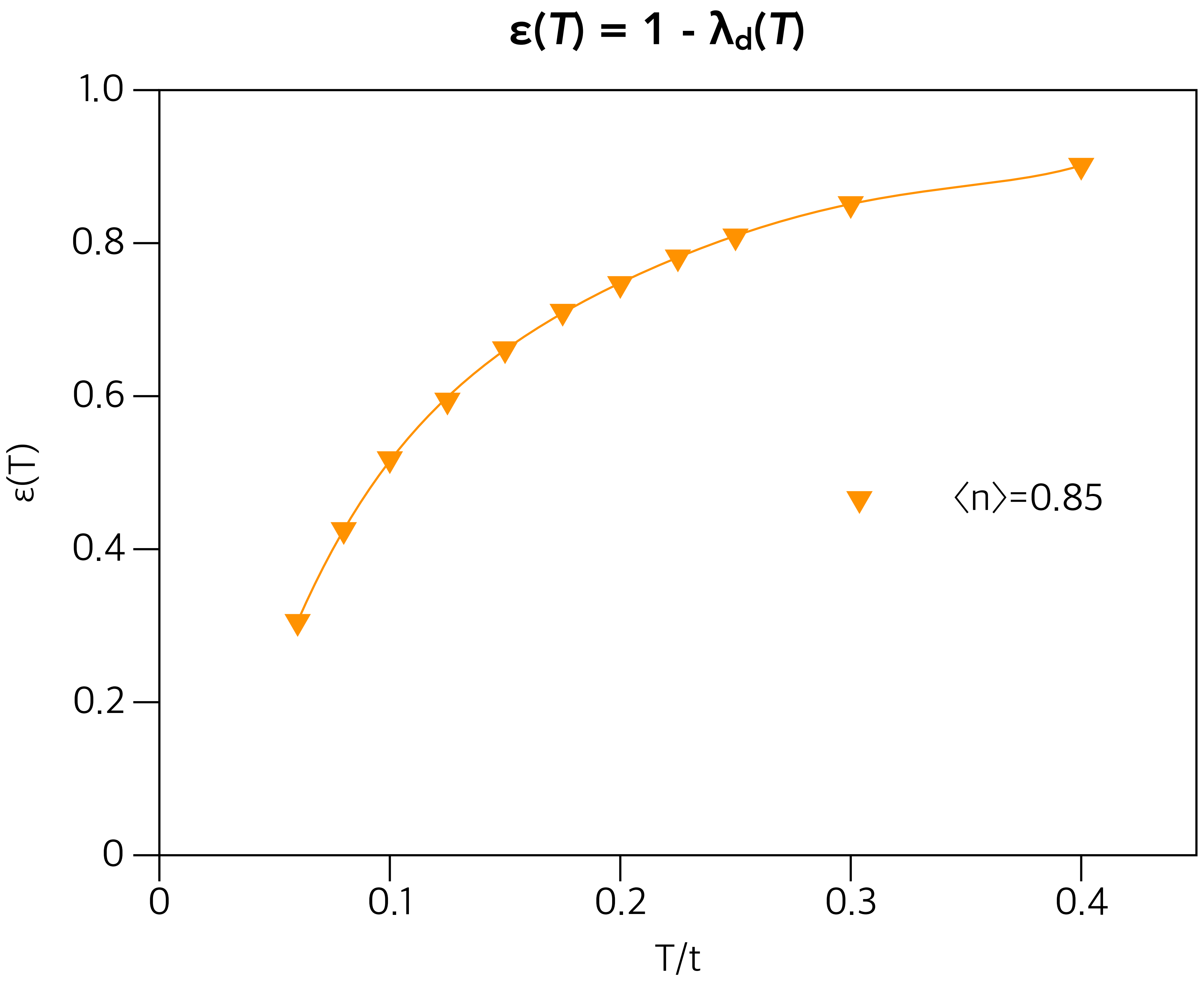


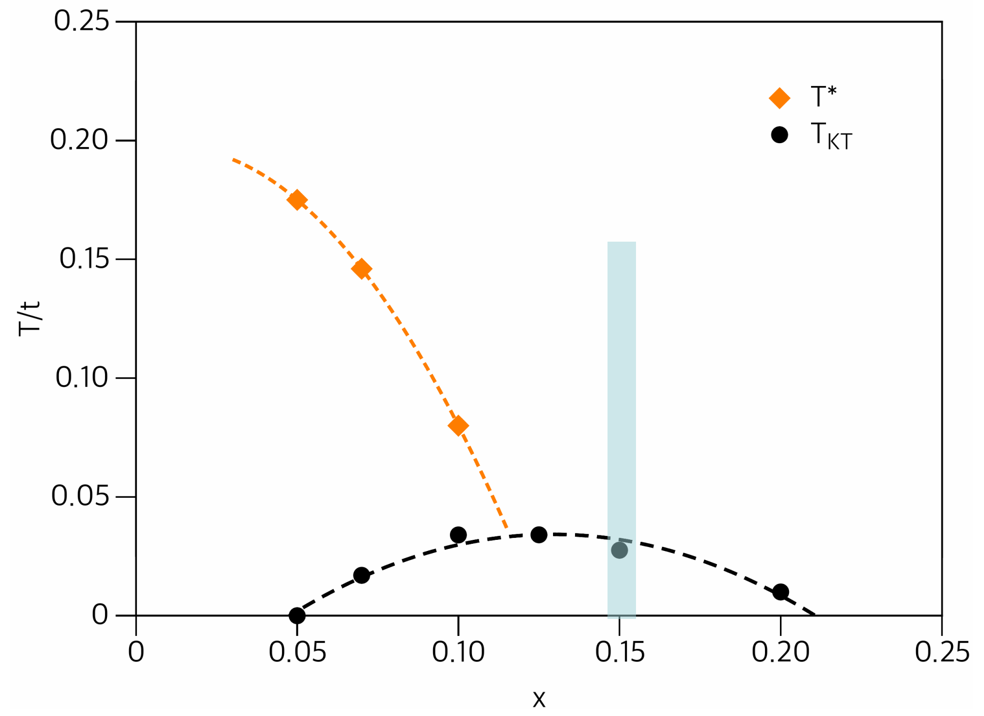
*Emery and S.A. Kivelson, Nature **374**, 434 (1995)*

Doping dependence of $\varepsilon(T) = 1 - \lambda_d(T)$

$$P_d(T) = \frac{P_{d,0}(T)}{1 - \lambda_d(T)}$$







TAM & Scalapino, npj Quant. Mat. ‘19

Doping dependence of ε(T)

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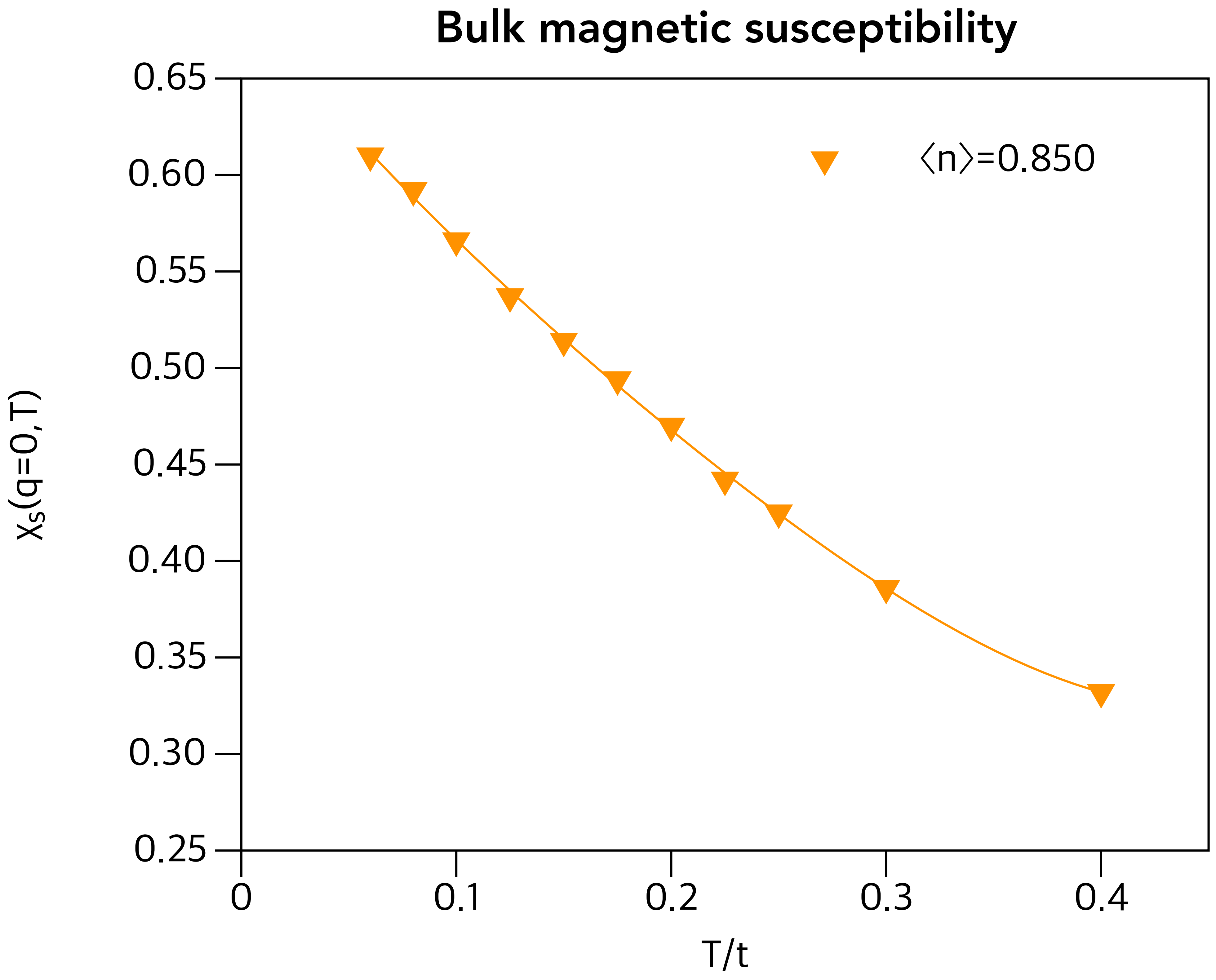

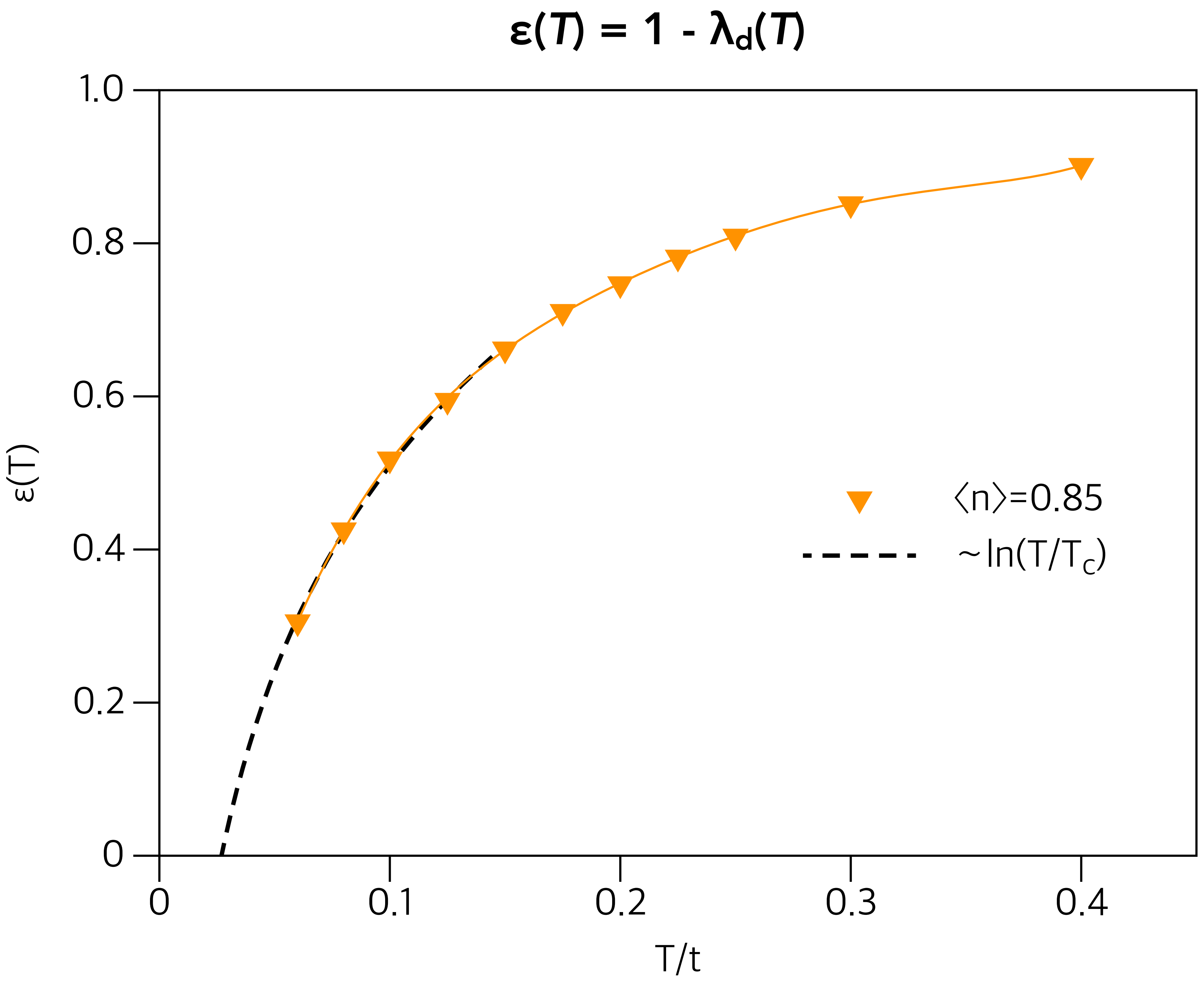

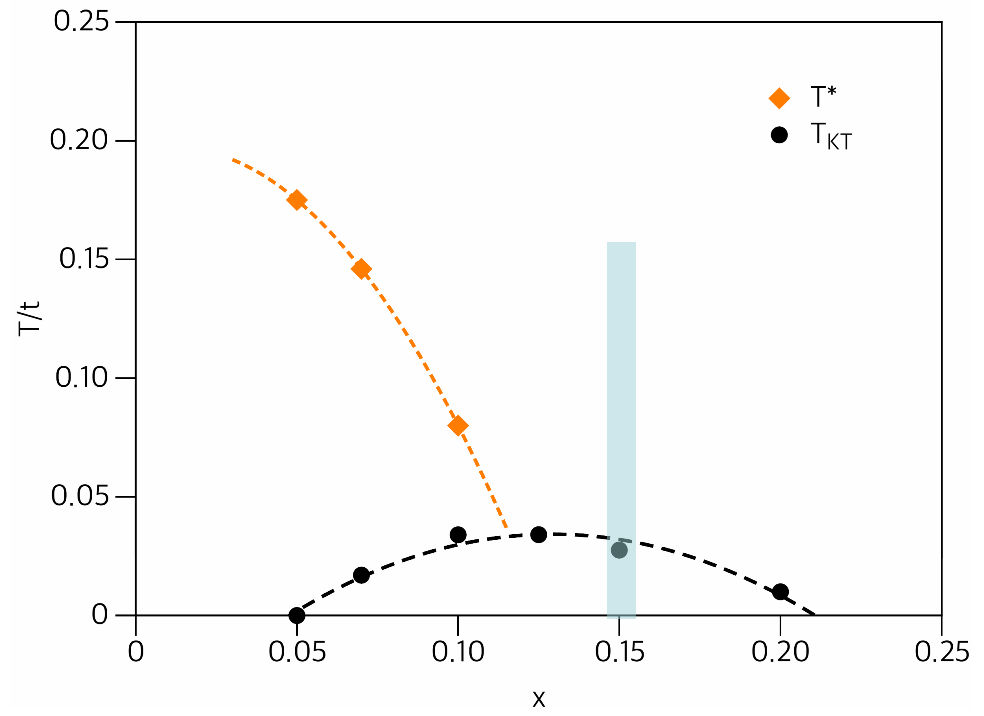

TAM & Scalapino, npj Quant. Mat. '19

Overdoped region

$$\varepsilon(T) \sim \ln(T/T_c^{\mathrm{MF}})$$

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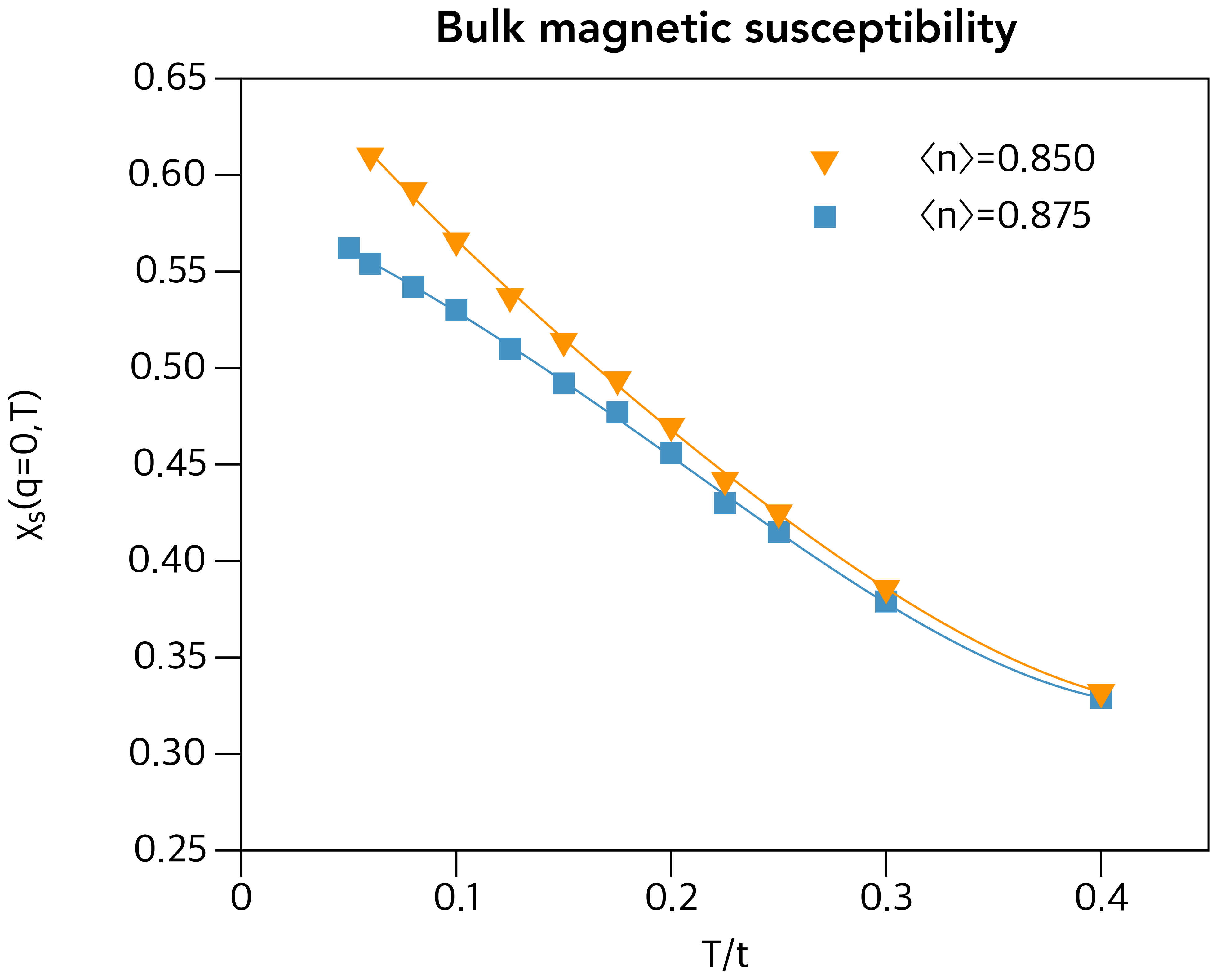

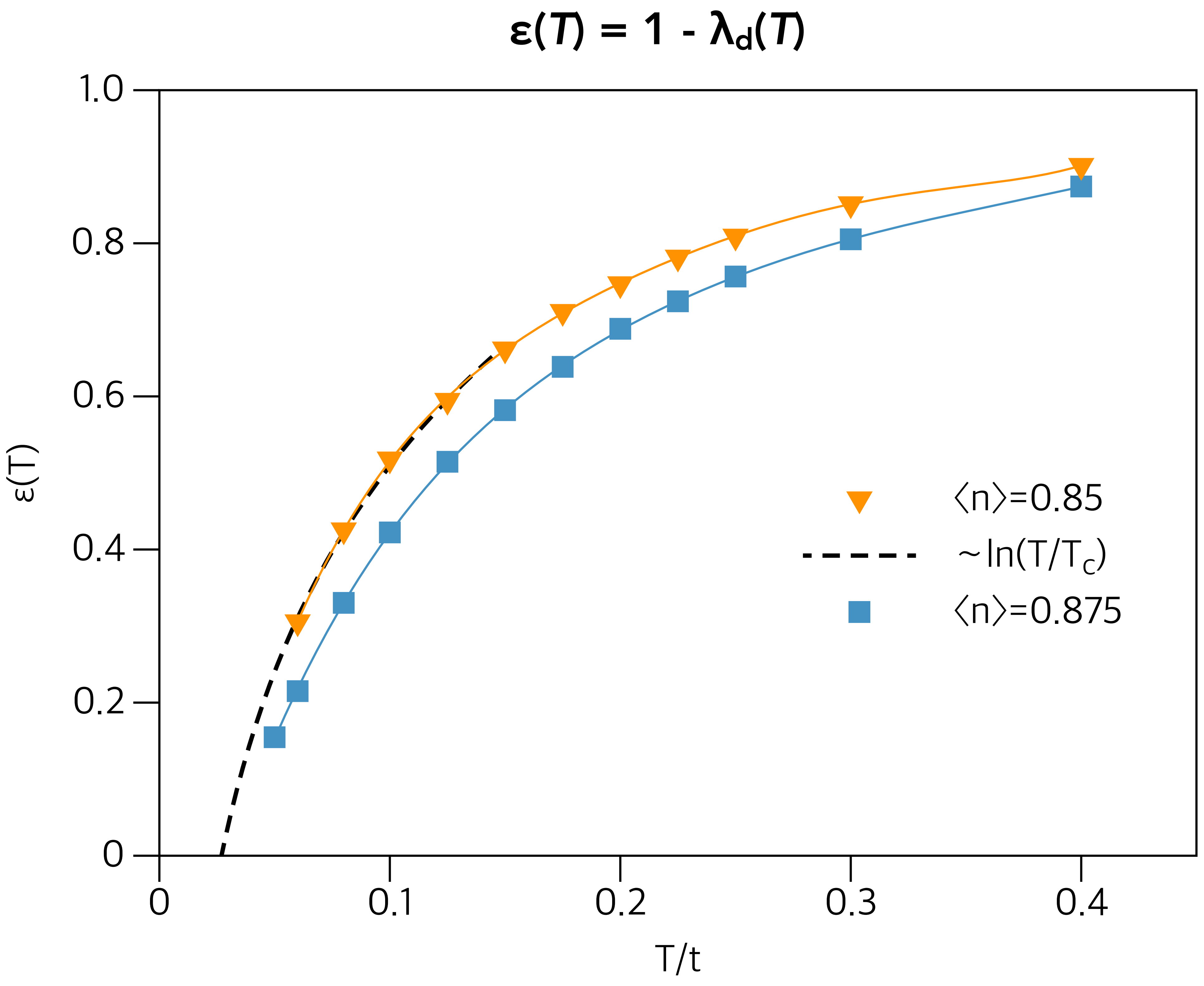

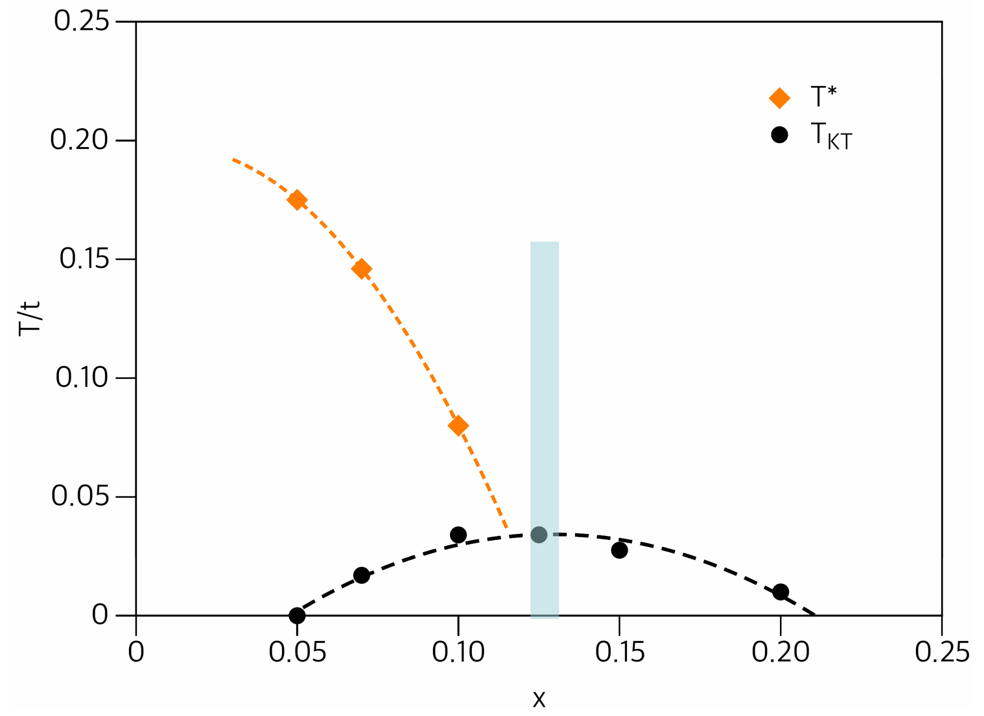

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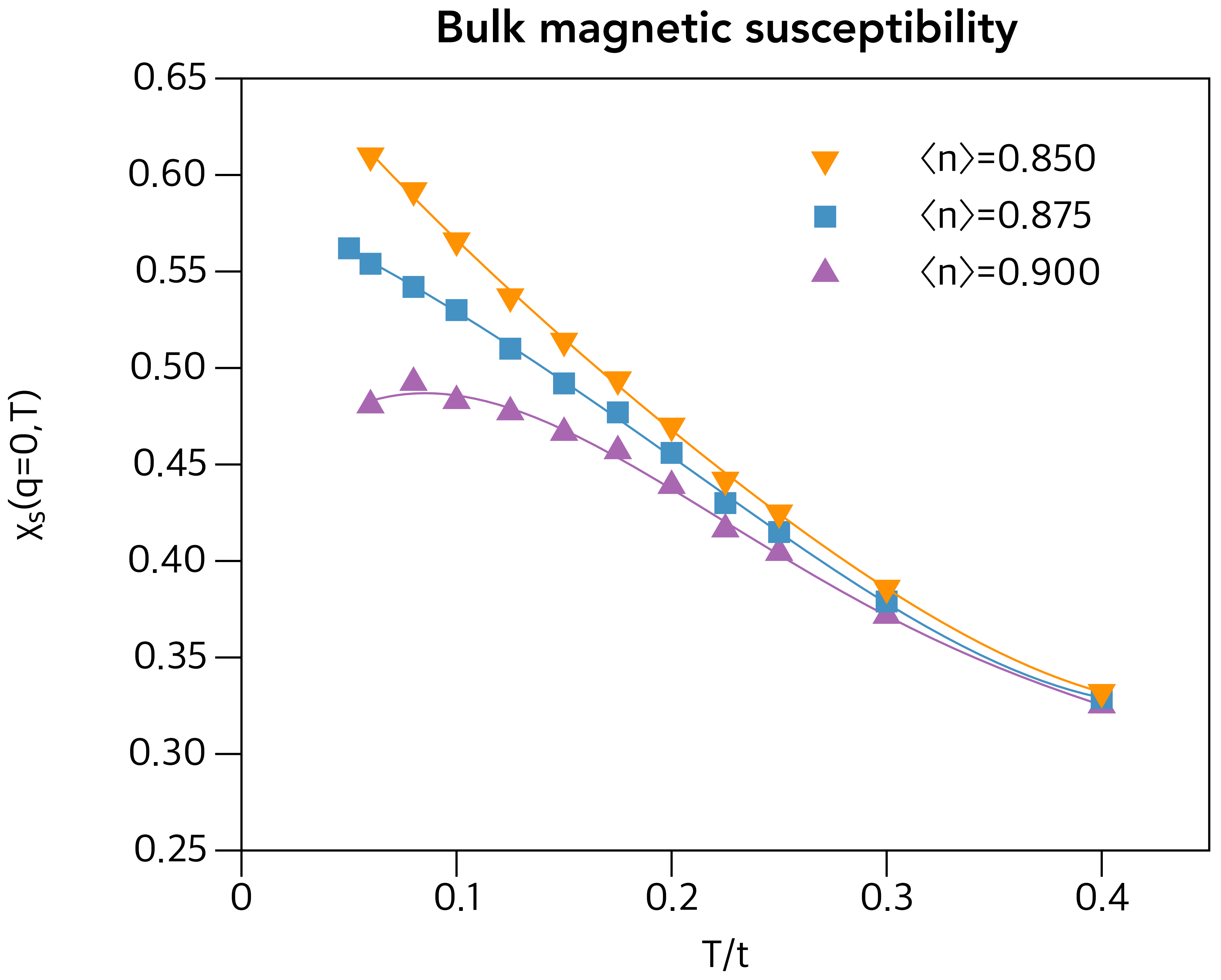

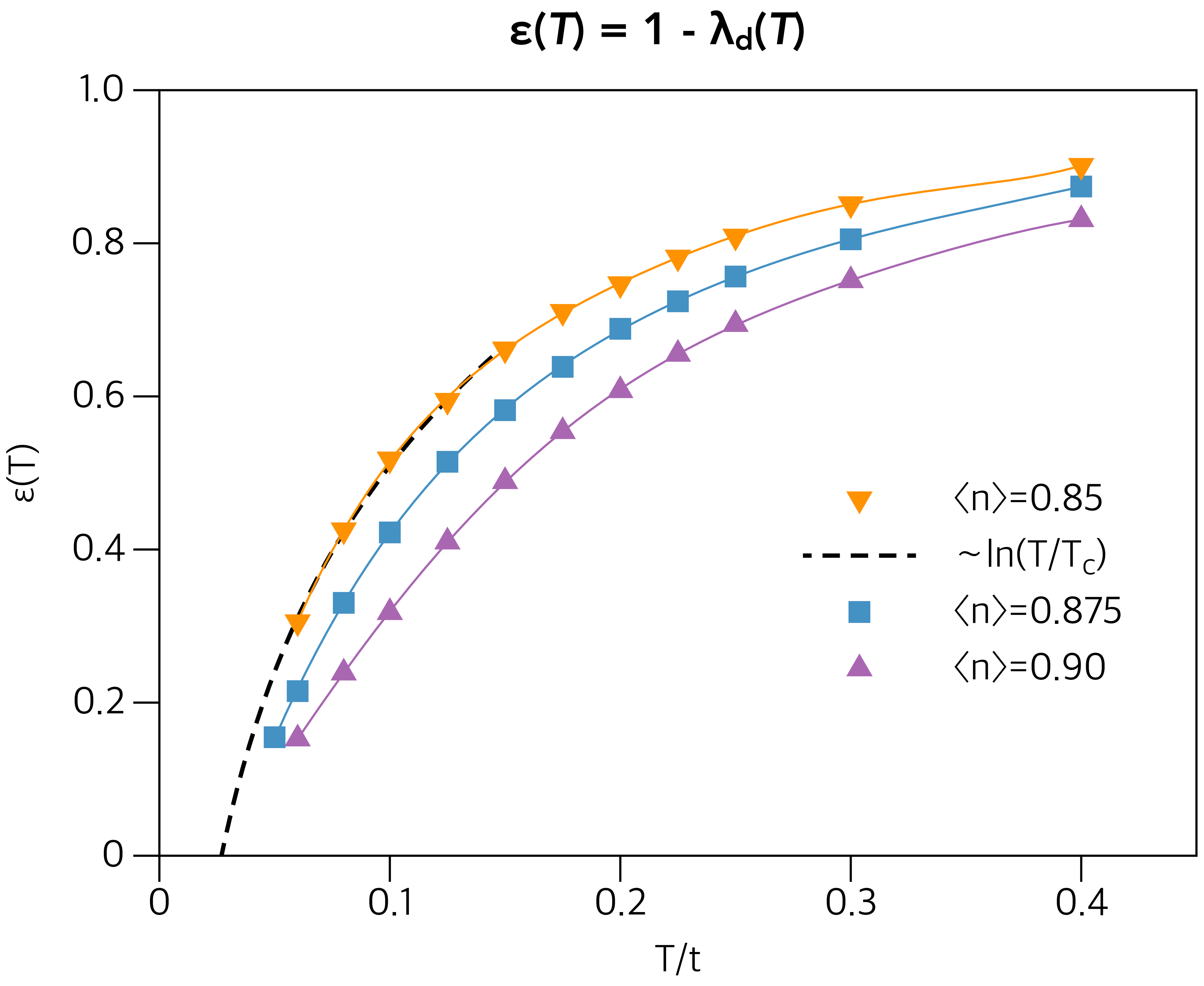

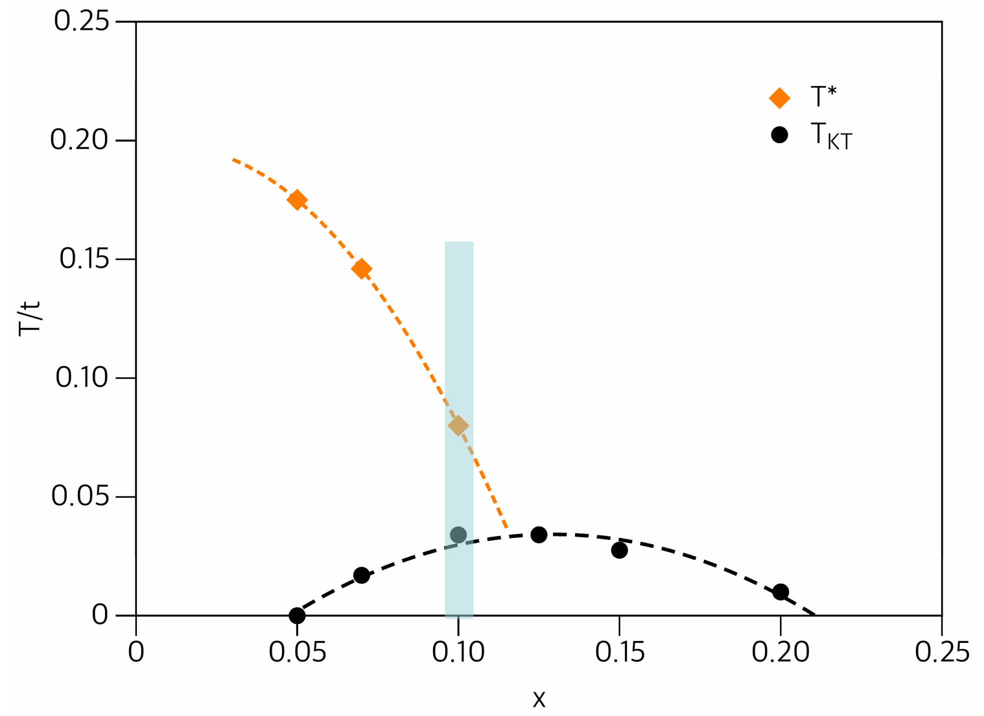

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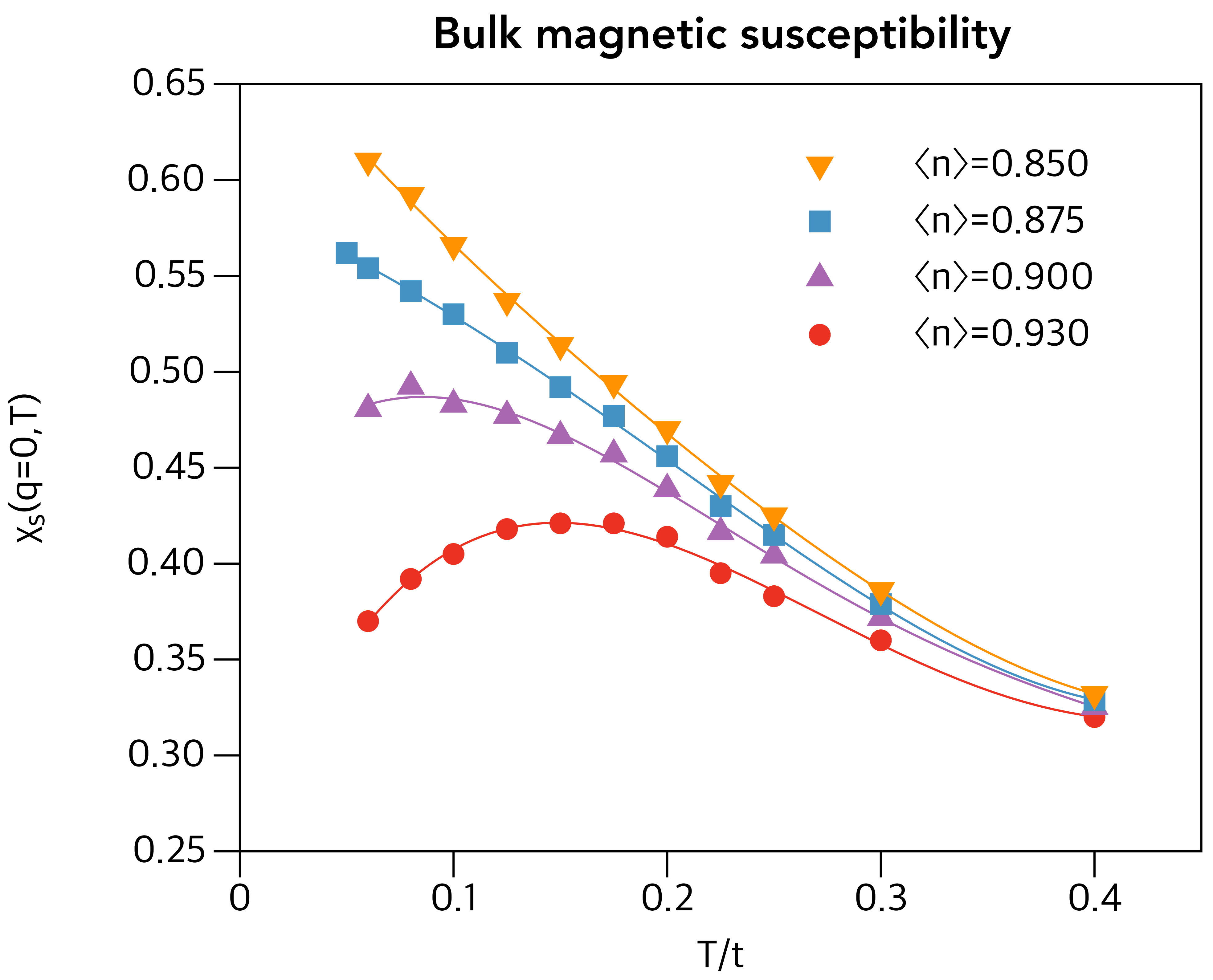
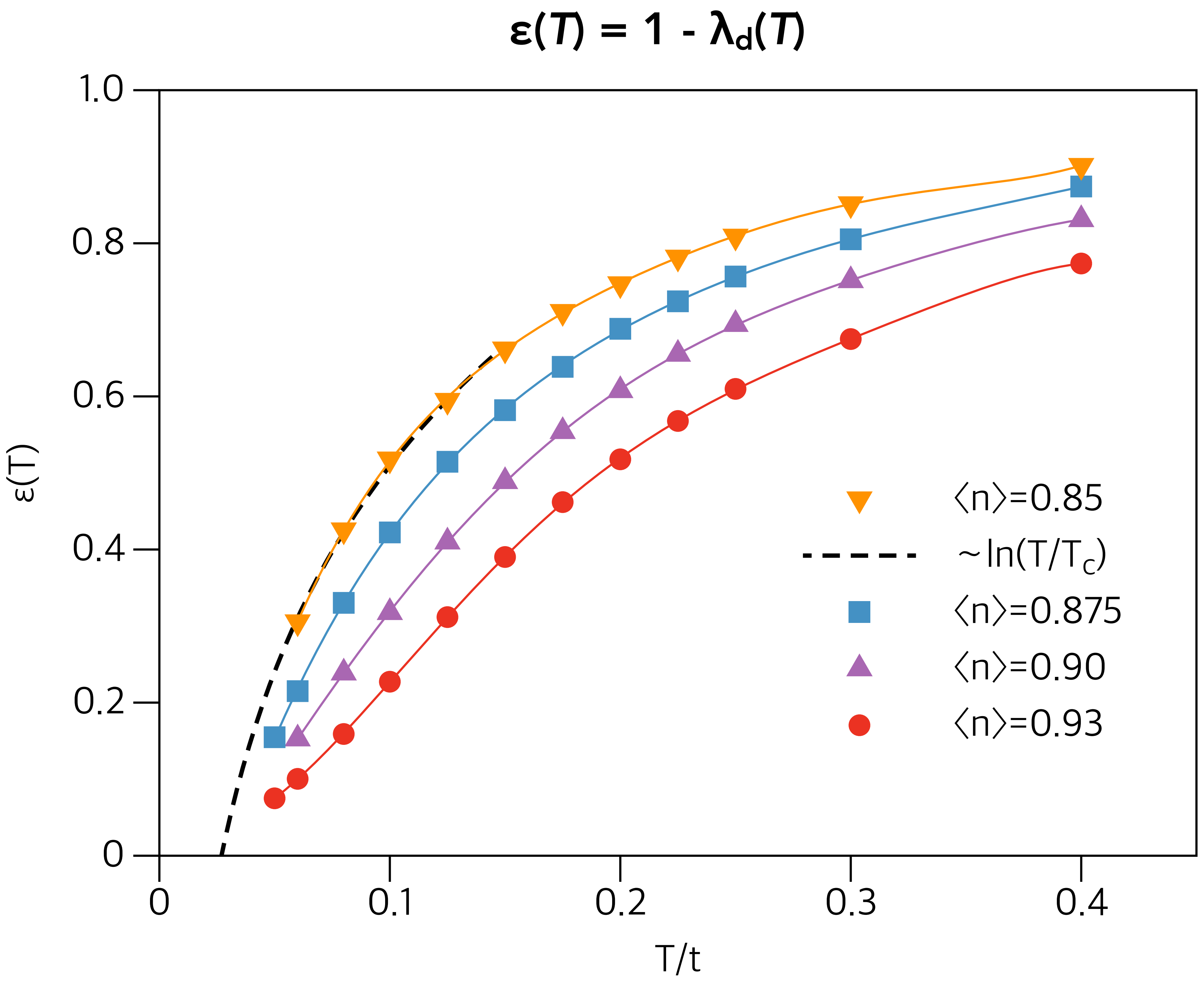
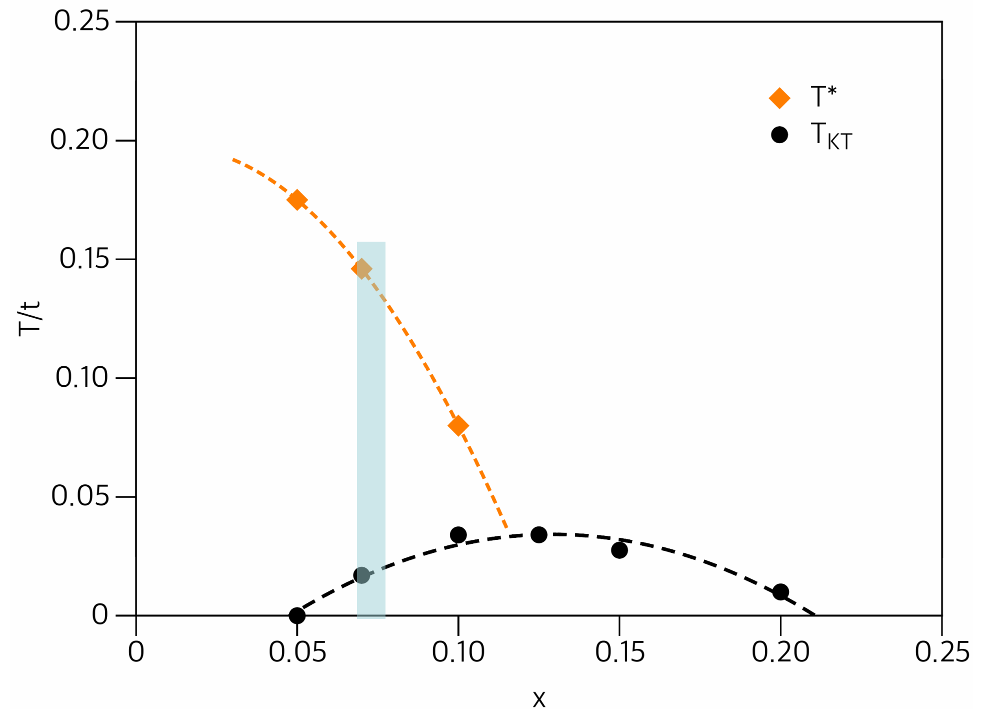




⇒ Pseudogap in underdoped region



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TAM & Scalapino, npj Quant. Mat. '19

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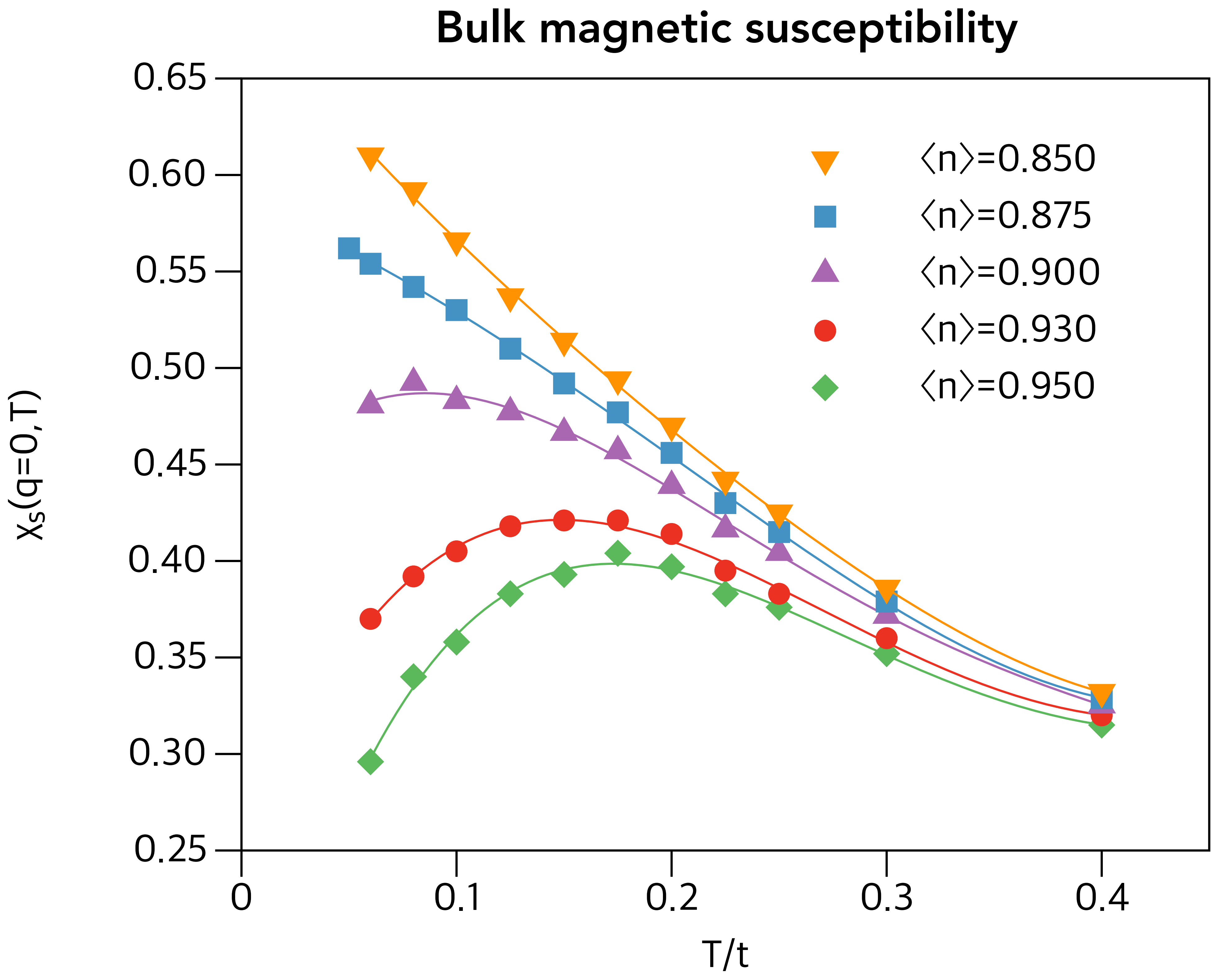
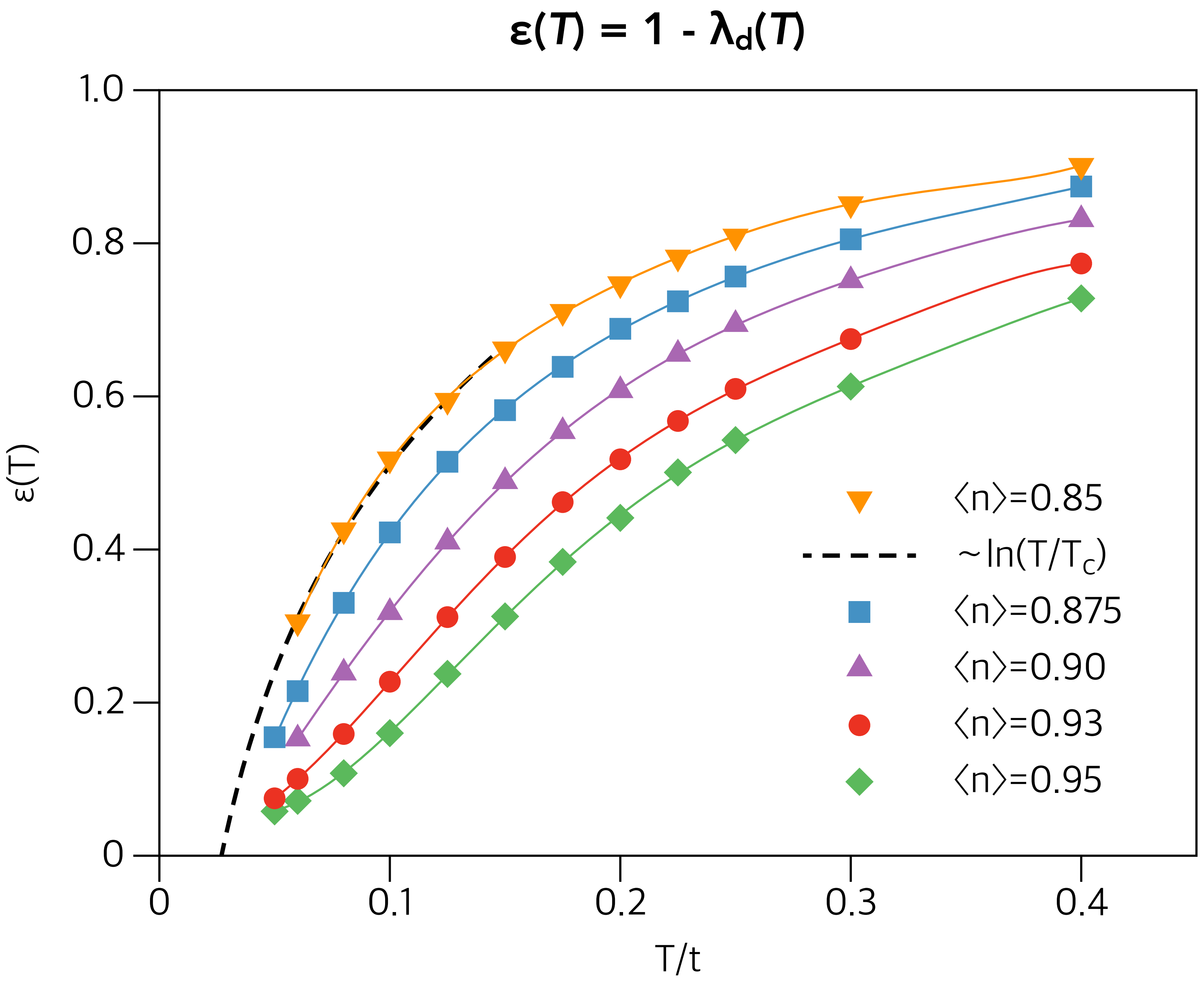
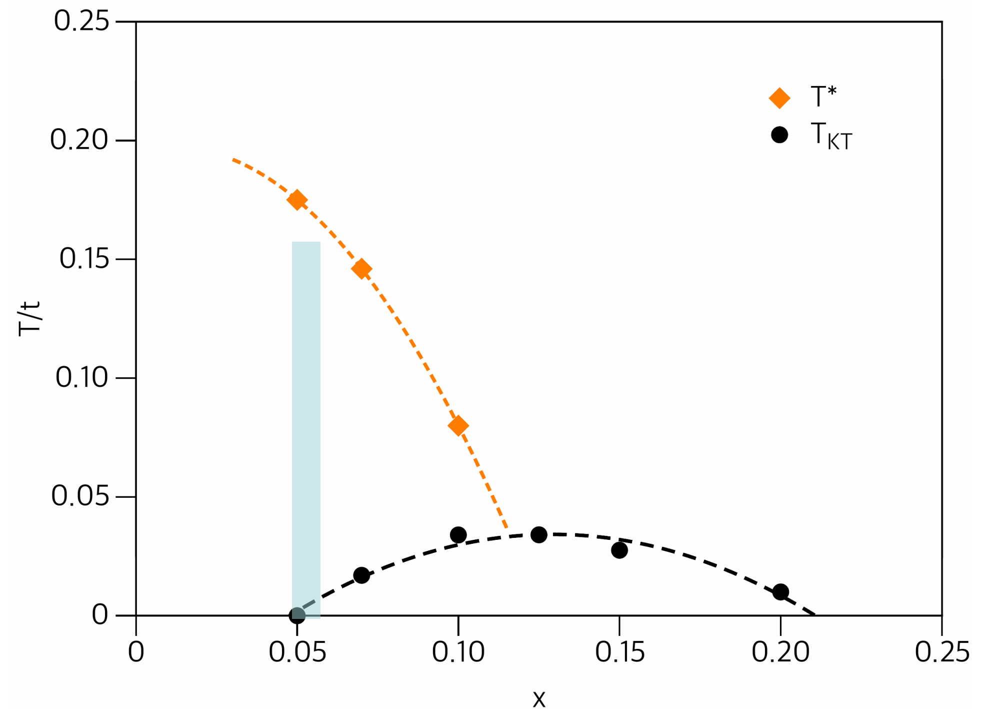




⇒ **Pseudogap in underdoped region**

TAM & Scalapino, npj Quant. Mat. '19



Overdoped region

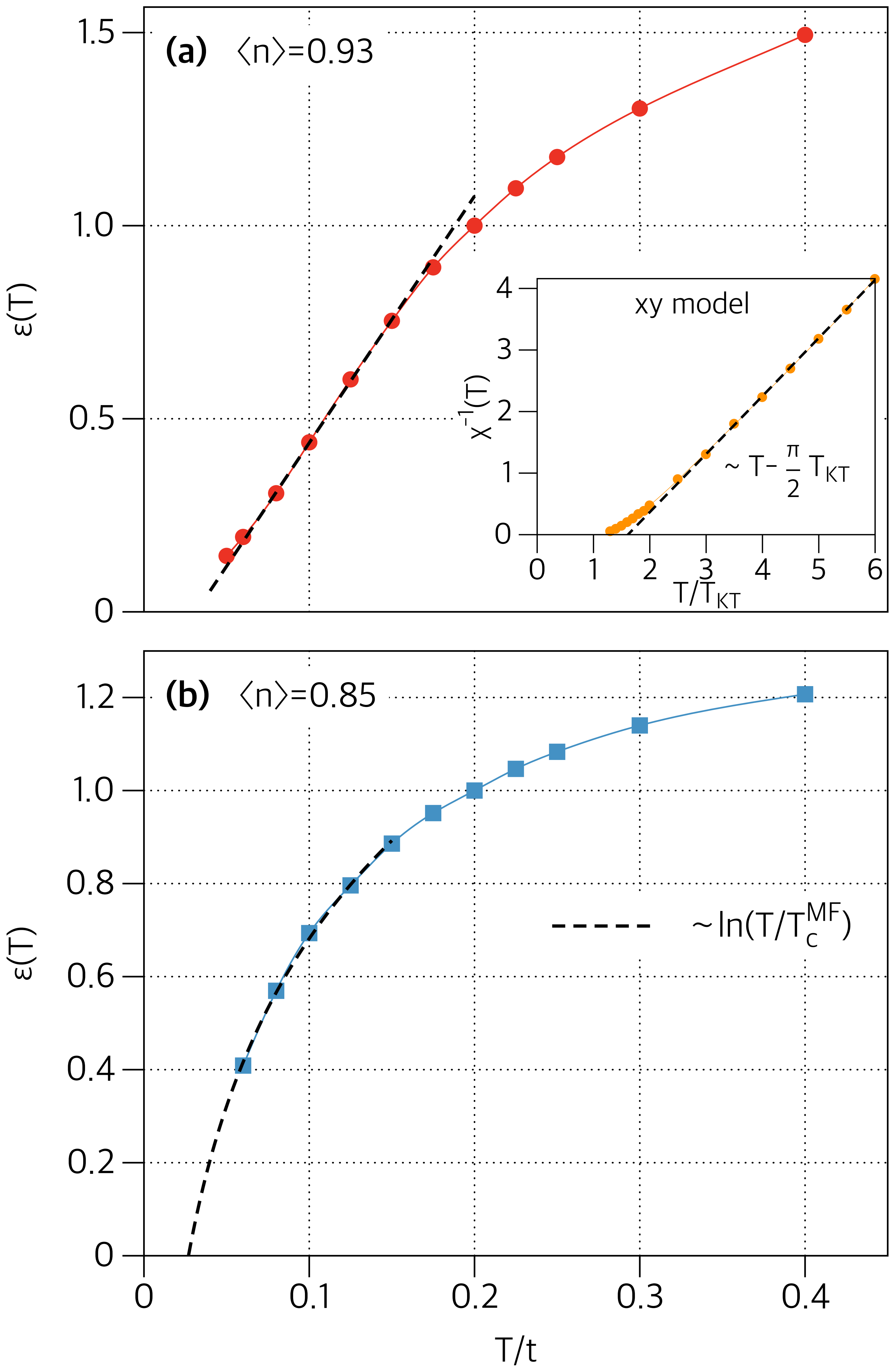
$$\varepsilon(T) \sim \ln(T/T_c^{\mathrm{MF}})$$

Underdoped region

$$\varepsilon(T) \sim T - \frac{\pi}{2} T_{\mathrm{KT}}$$

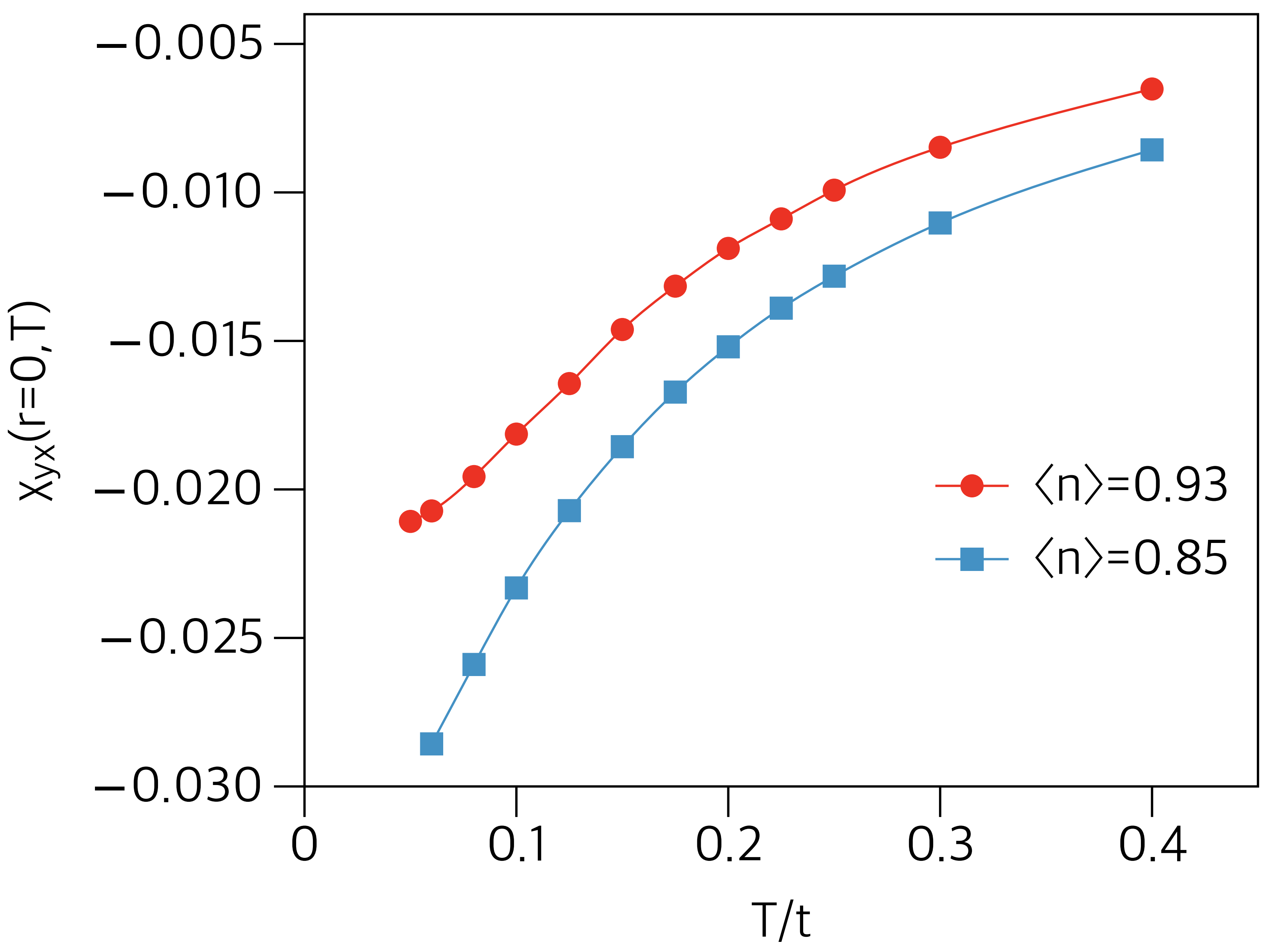
$$\varepsilon(T) \sim e^{-\frac{B}{\sqrt{|T - T_{\mathrm{KT}}|}}}$$

Phase fluctuations in underdoped pseudogap region



Local pair-field:

$$\chi_{yx}(r=0,T) = \frac{1}{N}\sum_{\ell}\int_0^{\beta} d\tau \, \langle \Delta_{\ell+y,\ell}(\tau)\Delta^{\dagger}_{\ell+x,\ell}(0)\rangle$$



- **Amplitude of local pair-field limited by opening of pseudogap**
- **Increase in pairfield susceptibility reflects increase in phase coherence**

TAM & Scalapino, npj Quant. Mat. '19

OAK RIDGE National Laboratory

This can be measured!

PAIR TUNNELING AS A PROBE OF FLUCTUATIONS IN SUPERCONDUCTORS*

D. J. Scalapino
Department of Physics, University of California, Santa Barbara, California 93106
(Received 10 March 1970)

Junction pair tunneling current

$$\langle I(V)\rangle = c\Delta_d P_d''(\omega = 2eV)$$

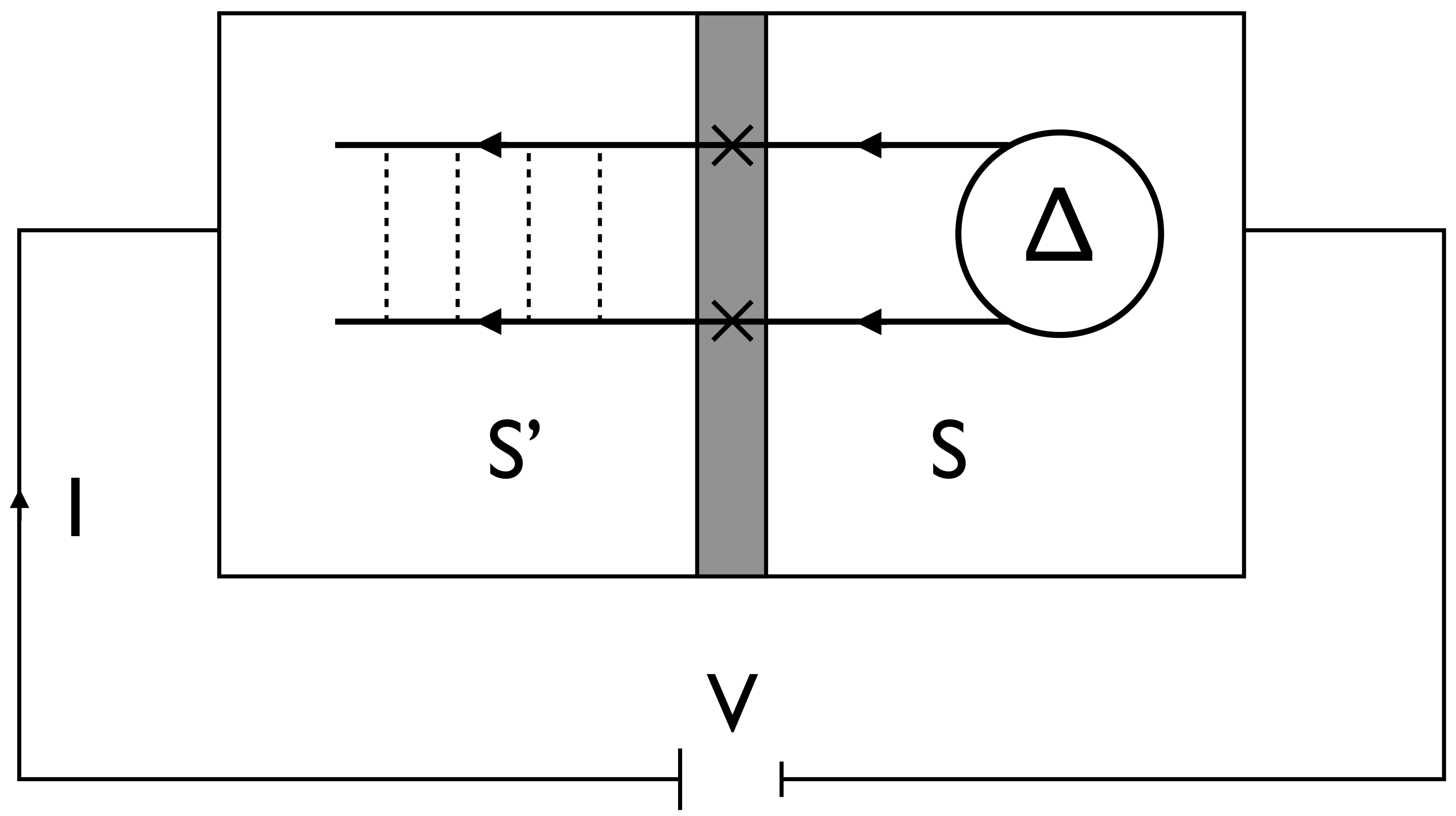
Ginzburg-Landau (ladder) approximation

$$P_d(\omega) \sim \frac{1}{\epsilon(T) - \frac{i\omega}{\Gamma_0}}\,;\;\; \epsilon(T) = 1 - \lambda_d(T)\,;\;\; \Gamma_0 = 8T_c/\pi$$

$$I(V) \sim P_d''(\omega = 2eV) \sim \frac{\frac{2eV}{\Gamma_0}}{\epsilon^2 + \left(\frac{2eV}{\Gamma_0}\right)^2}$$

Generally

$$P_d(\omega = 0, T) = \frac{P_{d,0}(T)}{1 - \lambda_d(T)} \sim \int dV\, I(V)/V$$



Tunnel junction between S and S′ with $T_c(S) < T < T_c(S')$

*Scalapino, PRL **24**, 1052 (1970)*
*Ferrell, Low Temp. Phys. **1**, 423 (1969)*

This can be measured!

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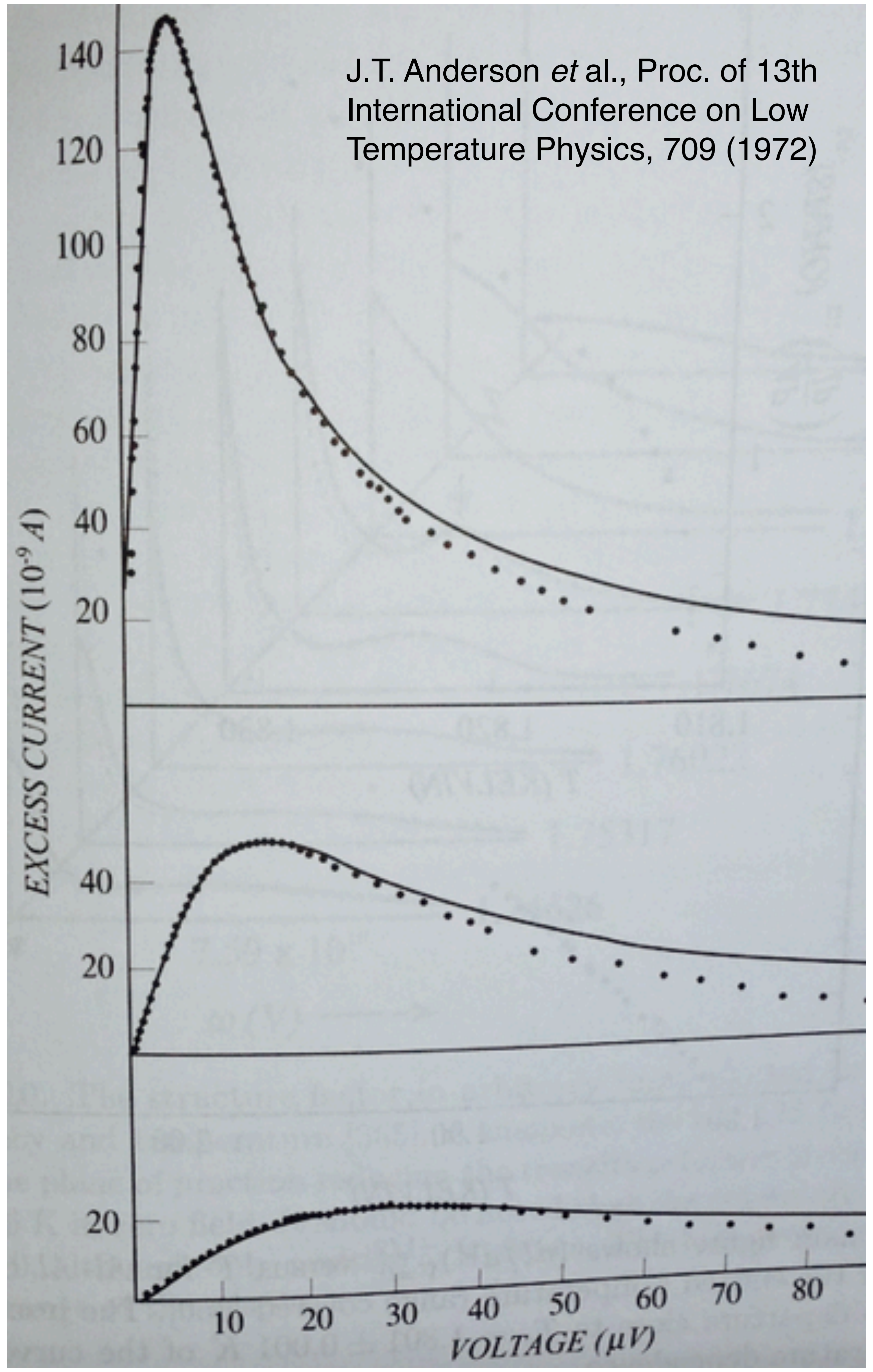

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Superconductivity in 2D Hubbard Model: Summary

- ***Cluster dynamical mean field theory*** finds robust ***d-wave superconductivity in the doped 2D Hubbard model*** (as well as a pseudogap)
- The ***pairing interaction carries spin S=1***, increases with momentum transfer, and its dynamics reflects the ***spin fluctuation*** spectrum
- In the ***overdoped region***, the superconducting instability arises from the conventional ***Cooper log divergence*** of the pair propagator
- In the ***underdoped pseudogap region***, the ***Cooper log instability is absent***, and superconductivity arises from an ***increase in the pairing interaction*** as the temperature is lowered and the ***development of long range phase coherence***

Acknowledgments

Early work

- Mark Jarrell
- Thomas Pruschke
- Joachim Keller

CompFUSE SciDAC Team (ORNL / LANL / UTK / UCSB / UFL):

- Gonzalo Alvarez
- Matthew Bachstein
- Feng Bao
- Tom Berlijn
- Arghya Chatterjee
- Ed D'Azevedo
- Philip Dee
- Peter Doak
- Wael Elwasif
- Oscar Hernandez
- Steve Johnston
- Seher Karakuzu
- Aaron Kirby
- Pontus Laurell
- Ying Wai Li
- Peizhi Mai
- Satoshi Okamoto
- Doug Scalapino
- Clayton Webster
- Xuping Xie

ETH Zürich

- Giovanni Balduzzi
- Urs Hähner
- Thomas Schulthess
- Peter Staar